# **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.

```
svms 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) ];
```

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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 <a href="mailto:symbolic\_functions.c">symbolic\_functions.c</a>.

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

#### 2.1.7 Initial Conditions

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

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

## 2.1.8 Observables

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

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

In the definition of the observable you can use certain symbolic functions. For a full list of available functions see <a href="mailto:symbolic\_functions.c">symbolic\_functions.c</a>. 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.y = 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 Model Simulation 7

#### 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:

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

The NaN values in Sigma\_Y and Sigma\_T will be replaced by the specification in Standard Deviation. Data points with NaN value will be completely ignored.

Generate a constants vector:

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

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

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

## 2.3.4 Steady State Sensitivities

This will compute state sensitivities according to the formula  $s_k^x = -\left(\frac{\partial f}{\partial x}\right)^{-1}\frac{\partial f}{\partial \theta_k}$ 

In the current implementation this formulation does not allow for conservation laws as this would result in a singular Jacobian.

Define a final timepoint t:

```
t = 100
```

Generate a parameter vector:

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

Generate a constants vector:

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

Set the sensitivity computation to steady state sensitivities:

3 Code Organization

```
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 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.

### 4 Class Index

### 4.1 Class List

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

#### amimodel

Amimodel is the object in which all model definitions are stored

ExpData	
Struct that carries all information about experimental data	22
ReturnData	
Struct that stores all data which is later returned by the mex function	22
TempData	
Struct that provides temporary storage for different variables	24
UserData	
Struct that stores all user provided data	26

## 5 Class Documentation

#### 5.1 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

 mlhsInnerSubst< matlabtypesubstitute > writeCcode (::string funstr,::fileid fid, matlabtypesubstitute ip, matlabtypesubstitute ip)

writeCcode is a wrapper for this.gccode which initialises data and reduces overhead by check nonzero values

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

 $\bullet \ \ mlhs Inner Subst < matlab type substitute > gccode \ (::symbolic \ csym, ::string \ funstr, ::string \ cvar, ::fileid \ fid) \\$ 

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 >> check-Deps (::struct HTable,::cell deps)

checkDeps checks the dependencies of functions and populates sym fields if necessary

 mlhsSubst< mlhsInnerSubst< matlabtypesubstitute >>,mlhsInnerSubst< matlabtypesubstitute >> loadOld-Hashes ()

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

### 5.1.1 Detailed Description

Definition at line 17 of file amimodel.m.

## 5.1.2 Constructor & Destructor Documentation

## 5.1.2.1 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 279 of file amimodel.m.

## 5.1.3 Member Function Documentation

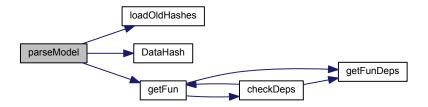
## 5.1.3.1 mlhslnnerSubst<::amimodel > parseModel ( )

Return values

this	updated model definition object

Definition at line 18 of file parseModel.m.

Here is the call graph for this function:



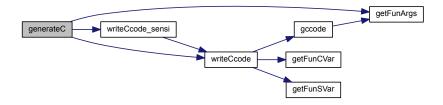
## 5.1.3.2 mlhsInnerSubst<::amimodel > generateC ( )

### Return values

this	model definition object

Definition at line 18 of file generateC.m.

Here is the call graph for this function:



## 5.1.3.3 mlhslnnerSubst<::amimodel > compileC ( )

## Return values

this	model definition object

Definition at line 18 of file compileC.m.

## 5.1.3.4 mlhslnnerSubst<::amimodel > writeCcode\_sensi ( ::symbolic svar, ::fileid fid )

## **Parameters**

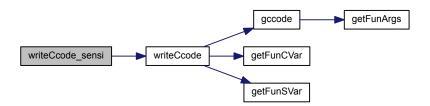
svar	symbolic variable which is later on passed to ggode
fid	file id in which the final expression is written

### 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:



5.1.3.5 mlhslnnerSubst<:::amimodel > writeCcode ( ::string funstr, ::fileid fid, matlabtypesubstitute ip, matlabtypesubstitute jp )

### **Parameters**

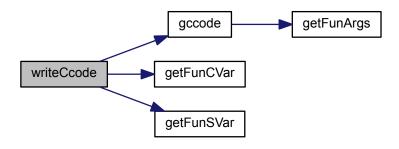
funstr	function for which C code is to be generated
fid	file id in which the final expression is written
ip	index for symbolic variable, if applicable svar(:,ip) will be passed to ggcode
јр	index for symbolic variable, if applicable svar(:,ip,jp) will be passed to ggcode

### Return values

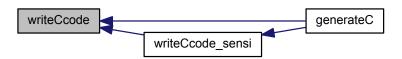
this	model definition object

Definition at line 18 of file writeCcode.m.

Here is the call graph for this function:



Here is the caller graph for this function:



## $5.1.3.6 \quad \text{mlhsInnerSubst} < \text{::amimodel} > \text{gccode} \ ( \ \text{::symbolic} \ \textit{csym}, \ \text{::string} \ \textit{funstr}, \ \text{::string} \ \textit{cvar}, \ \text{::fileid} \ \textit{fid} \ )$

### **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:



## $5.1.3.7 \quad \text{mlhsInnerSubst} < :: a mimodel > \text{generateM} \ ( \ :: a mimodel \ a mimodelo2 \ )$

### **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.

5.1.3.8 mlhslnnerSubst<::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**

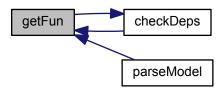
this	updated model definition object

Definition at line 18 of file getFun.m.

Here is the call graph for this function:



Here is the caller graph for this function:



## 5.1.3.9 mlhsInnerSubst<::cell > getFunDeps ( ::string funstr )

## **Parameters**

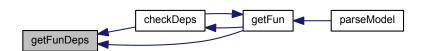
, ,	
funstr	function or expression for which the dependencies should be returned
7011011	Tarrottori or expression for which the dependencies chedia so retarried

### Return values

deps	cell array of dependencies

Definition at line 18 of file getFunDeps.m.

Here is the caller graph for this function:



## 5.1.3.10 mlhsInnerSubst< matlabtypesubstitute > getFunArgs ( ::string funstr )

#### **Parameters**

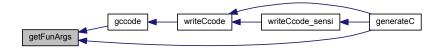
funstr	function name

### **Return values**

str	string containing function arguments

Definition at line 18 of file getFunArgs.m.

Here is the caller graph for this function:



## 5.1.3.11 mlhsInnerSubst<::string > getFunCVar (::string funstr)

#### **Parameters**

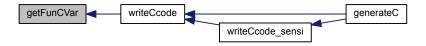
funstr	function or expression for which the dependencies should be returned

### Return values

cvar	cell array of dependencies

Definition at line 18 of file getFunCVar.m.

Here is the caller graph for this function:



## 5.1.3.12 mlhsInnerSubst < matlabtypesubstitute > getFunSVar (::string funstr)

## **Parameters**

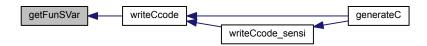
funstr	function or expression for which the dependencies should be returned
--------	--

#### **Return values**

cvar	cell array of dependencies

Definition at line 18 of file getFunSVar.m.

Here is the caller graph for this function:



5.1.3.13 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:



## $5.1.3.14 \quad mlhs Subst < mlhs Inner Subst < :: a mimodel > , mlhs Inner Subst < :: struct > > load Old Hashes ( \ \ )$

## 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:



5.1.3.15 mlhslnnerSubst<::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.

5.1.4 Member Data Documentation

5.1.4.1 atol = 1e-8

Default: 1e-8

Definition at line 61 of file amimodel.m.

5.1.4.2 rtol = 1e-8

Default: 1e-8

Definition at line 69 of file amimodel.m.

5.1.4.3 maxsteps = 1e4

Default: 1e4

Definition at line 77 of file amimodel.m.

5.1.4.4 debug = false

Default: false

Definition at line 85 of file amimodel.m.

5.1.4.5 adjoint = true

Default: true

Definition at line 93 of file amimodel.m.

5.1.4.6 forward = true

Default: true

Definition at line 101 of file amimodel.m.

 $5.1.4.7 \quad t0 = 0$ 

Default: 0

Definition at line 109 of file amimodel.m.

5.1.4.8 nxtrue = 0

Default: 0

Definition at line 131 of file amimodel.m.

```
5.1.4.9 nytrue = 0
```

### Default: 0

Definition at line 146 of file amimodel.m.

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

## Default: "-O3"

Definition at line 259 of file amimodel.m.

```
5.1.4.11 param = "lin"
```

## Default: "lin"

Definition at line 267 of file amimodel.m.

## 5.2 ExpData Struct Reference

struct that carries all information about experimental data

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

## **Public Attributes**

double \* am\_my

observed data

• double \* am\_ysigma

standard deviation of observed data

double \* am mt

observed events

double \* am\_tsigma

standard deviation of observed events

## 5.2.1 Detailed Description

Definition at line 18 of file edata.h.

## 5.3 ReturnData Struct Reference

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

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

### **Public Attributes**

• double \* am\_tsdata

timepoints

• double \* am\_xdotdata

time derivative

• double \* am\_dxdotdpdata

parameter derivative of time derivative

```
    double * am_dydxdata

     state derivative of observables

    double * am_dydpdata

     parameter derivative of observables
double * am_Jdata
     Jacobian of differential equation right hand side.
• double * am rootdata
     events
double * am_rootSdata
     parameter derivative of events
double * am_rootS2data
     second order parameter derivative of events
double * am_rootvaldata
      value of event function

    double * am rootvalSdata

     parameter derivative of event function
double * am_rootvalS2data
     second order parameter derivative of event function
double * am_xdata
     state

    double * am xSdata

     parameter derivative of state
double * am_ydata
     observable
double * am_ySdata
     parameter derivative of observable
• double * am_numstepsdata
     number of integration steps forward problem

    double * am_numstepsSdata

     number of integration steps backward problem
• double * am_numrhsevalsdata
     number of right hand side evaluations forward problem

    double * am_numrhsevalsSdata

     number of right hand side evaluations backwad problem
• double * am_orderdata
     employed order forward problem

    double * am_llhdata

     likelihood value
• double * am chi2data
     chi2 value
• double * am_llhSdata
     parameter derivative of likelihood
• double * am_llhS2data
     second order parameter derivative of likelihood
```

### 5.3.1 Detailed Description

Definition at line 42 of file rdata.h.

```
5.3.2 Member Data Documentation
5.3.2.1 double * am_xdata
returned vector
Definition at line 69 of file rdata.h.
      TempData Struct Reference
struct that provides temporary storage for different variables
#include <tdata.h>
Public Attributes
    • realtype am_t
          current time
    • N_Vector am_x
          state vector

    N_Vector am_dx

          differential state vector

    N_Vector am_xdot

          time derivative state vector

    N_Vector am_xB

          adjoint state vector

    N_Vector am_dxB

          differential adjoint state vector

    N_Vector am_xQB

          quadrature state vector
    N_Vector * am_sx
          sensitivity state vector array
    N_Vector * am_sdx
          differential sensitivity state vector array

    N_Vector am_id

          index indicating DAE equations vector
    · DIsMat am_Jtmp
          Jacobian.
    double * am_IIhS0
          parameter derivative of likelihood array
    • double am_g
          data likelihood
    double * am_dgdp
          parameter derivative of data likelihood
    double * am_dgdx
          state derivative of data likelihood
    · double am_r
          event likelihood
    double * am_drdp
          parameter derivative of event likelihood
    double * am_drdx
```

state derivative of event likelihood

```
    double am_rval

     root function likelihood

    double * am drvaldp

     parameter derivative of root function likelihood

    double * am drvaldx

     state derivative of root function likelihood
double * am_dtdx
     state derivative of event

    double * am dtdp

     parameter derivative of event
double * am_dydp
     parameter derivative of observable
double * am_dydx
     state derivative of observable

 double * am yS0

     initial sensitivity of observable

    double * am sigma y

     data standard deviation
double * am_dsigma_ydp
     parameter derivative of data standard deviation
double * am_sigma_t
     event standard deviation

    double * am_dsigma_tdp

     parameter derivative of event standard deviation

 double * am x tmp

     state array
double * am_sx_tmp
     sensitivity state array
double * am_dx_tmp
     differential state array
double * am_sdx_tmp
     differential sensitivity state array
double * am_xdot_tmp
     time derivative state array
double * am_xB_tmp
     differential adjoint state array
double * am_xQB_tmp
     quadrature state array
double * am_dxB_tmp
     differential adjoint state array
double * am_id_tmp
     index indicating DAE equations array
int * am_rootsfound
     array of flags indicating which root has beend found

    double * am_rootvaltmp

     array of values of the root function
int * am rootidx
     array of index which root has been found
int am_which
     integer for indexing of backwards problems
double * am_discs
     array containing the time-points of discontinuities

    double * am_irdiscs

     array containing the index of discontinuities
```

### 5.4.1 Detailed Description

Definition at line 64 of file tdata.h.

#### 5.4.2 Member Data Documentation

```
5.4.2.1 int* am_rootsfound
```

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.

## 5.5 UserData Struct Reference

struct that stores all user provided data

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

### **Public Attributes**

```
int * am_plist
```

parameter reordering

int am\_np

number of parameters

int am\_ny

number of observables

• int am\_nx

number of states

• int am\_nr

number of roots

• int am\_nt

number of timepoints

• int am\_ndisc

number of discontinuities

• int am\_nnz

number of nonzero entries in jacobian

• int am\_nmaxroot

maximal number of roots to collect

int am\_nmaxdisc

maximal number of discontinuities to track

double \* am\_p

parameter array

double \* am\_k

constants array

double am\_tstart

starting time

double \* am\_ts

timepoints

double \* am\_pbar

scaling of parameters

double \* am\_xbar

```
scaling of states
```

double \* am\_idlist

flag array for DAE equations

· int am sensi

flag indicating whether sensitivities are supposed to be computed

double am atol

absolute tolerances for integration

· double am\_rtol

relative tolerances for integration

• int am\_maxsteps

maximum number of allowed integration steps

• int am\_ism

internal sensitivity method

· int am\_sensi\_meth

method for sensitivity computation

• int am\_linsol

linear solver specification

int am\_interpType

interpolation type

• int am\_lmm

linear multistep method

· int am\_iter

nonlinear solver

• booleantype am\_stldet

flag controlling stability limit detection

· int am\_ubw

upper bandwith of the jacobian

• int am\_lbw

lower bandwith of the jacobian

booleantype am\_bsx0

flag for sensitivity initialisation

double \* am\_sx0data

sensitivity initialisation

int am\_event\_model

error model for events

int am\_data\_model

error model for udata

• int am\_ordering

state ordering

### 5.5.1 Detailed Description

Definition at line 61 of file udata.h.

#### 5.5.2 Member Data Documentation

## 5.5.2.1 int am\_ism

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 115 of file udata.h.

### 5.5.2.2 int am\_sensi\_meth

CW\_FSA for forward sensitivity analysis, CW\_ASA for adjoint sensitivity analysis

Definition at line 121 of file udata.h.

### 5.5.2.3 int am\_interpType

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 128 of file udata.h.

### 5.5.2.4 int am\_lmm

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

Definition at line 134 of file udata.h.

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

Definition at line 140 of file udata.h.

### 5.5.2.6 booleantype am\_bsx0

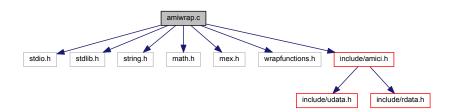
flag which determines whether analytic sensitivities initialisation or provided initialisation should be used Definition at line 154 of file udata.h.

## 6 File Documentation

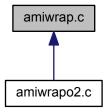
## 6.1 amiwrap.c File Reference

#### 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:



### **Functions**

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

### 6.1.1 Detailed Description

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

## 6.1.2 Function Documentation

6.1.2.1 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

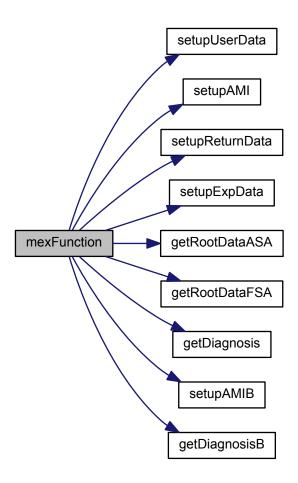
in	nlhs	number of output arguments of the matlab call
		Type: int
out	plhs	pointer to the array of output arguments
		Type: mxArray
in	nrhs	number of input arguments of the matlab call
		Type: int
in	prhs	pointer to the array of input arguments
		Type: mxArray

Returns

void

Definition at line 25 of file amiwrap.c.

Here is the call graph for this function:



## 6.2 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.

## 6.2.1 Function Documentation

6.2.1.1 noret::substitute amiwrap ( matlabtypesubstitute varargin )

#### **Parameters**

## varargin

1 amiwrap ( modelname, symfun, tdir, o2flag )

## Required Parameters for varargin:

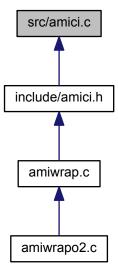
- modelname specifies the name of the model which will be later used for the naming of the simualation file
- symfun specifies a function which executes model defition see Model Definition for details
- tdir target directory where the simulation file should be placed **Default:** \$AMI-CIDIR/models/modelname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

Definition at line 17 of file amiwrap.m.

## 6.3 src/amici.c File Reference

core routines for integration

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



### Macros

• #define amici\_c

include guard

• #define AMI SUCCESS 0

return value indicating successful execution

#### **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)

#### 6.3.1 Function Documentation

#### 6.3.1.1 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 10 of file amici.c.

Here is the caller graph for this function:



6.3.1.2 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

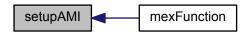
in	temp_data	pointer to the temporary data struct
		Type: TempData

### Returns

void

Definition at line 149 of file amici.c.

Here is the caller graph for this function:



6.3.1.3 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 434 of file amici.c.

Here is the caller graph for this function:



6.3.1.4 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

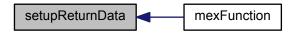
### Returns

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

user udata

Definition at line 625 of file amici.c.

Here is the caller graph for this function:



## 6.3.1.5 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 690 of file amici.c.

Here is the caller graph for this function:



6.3.1.6 void getRootDataFSA ( int \* status, int \* nroots, void \* ami\_mem, void \* user\_data, void \* return\_data, void \*  $temp\_data$  )

 ${\tt getRootDataFSA} \ {\tt extracts} \ {\tt root} \ {\tt information} \ {\tt for} \ {\tt forward} \ {\tt sensitivity} \ {\tt analysis}$ 

### **Parameters**

out	status	flag indicating success of execution
Ouc	Sidido	
		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 789 of file amici.c.

Here is the caller graph for this function:



6.3.1.7 void getRootDataASA ( int \* status, int \* nroots, int \* idisc, void \* ami\_mem, void \* user\_data, void \* return\_data, void \* exp\_data, void \* temp\_data )

 $getRootDataASA\ extracts\ root\ information\ for\ adjoint\ sensitivity\ analysis$ 

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 873 of file amici.c.

Here is the caller graph for this function:



6.3.1.8 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 981 of file amici.c.

Here is the caller graph for this function:



6.3.1.9 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 1015 of file amici.c.

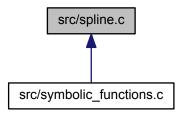
Here is the caller graph for this function:



# 6.4 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[])

#### 6.4.1 Detailed Description

### **Author**

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

#### 6.4.2 Function Documentation

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

#### Return values

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

# Notes

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

Definition at line 66 of file spline.c.

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

### Returns

the value of the spline function at u

#### Notes

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

Definition at line 208 of file spline.c.

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

### **Parameters**

in	n	the number of data points or knots (n $\geq$ = 2)
in	и	the abscissa at which the derivative is to be evaluated
in	X	the abscissas of the knots in strictly increasing order
in	b	array of spline coefficients computed by spline()
in	С	array of spline coefficients computed by spline()
in	d	array of spline coefficients computed by spline()

### Returns

the value of the derivative of the spline function at u

# Notes

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

Definition at line 264 of file spline.c.

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

### Returns

the value of the spline function at u

# Notes

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

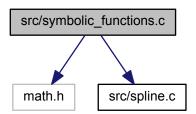
Definition at line 324 of file spline.c.

# 6.5 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
  - include guard
- #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 It (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)

### 6.5.1 Detailed Description

This file contains definitions of various symbolic functions which

### 6.5.2 Macro Definition Documentation

#### 6.5.2.1 #define TRUE 1

bool return value true

Definition at line 15 of file symbolic\_functions.c.

### 6.5.2.2 #define FALSE 0

bool return value false

Definition at line 17 of file symbolic\_functions.c.

#### 6.5.3 Function Documentation

### 6.5.3.1 int am\_ge ( double a, double b )

c implementation of matlab function ge

#### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

### Returns

if(a  $\geq$ = 0) then 1 else 0

Type: int

Definition at line 27 of file symbolic\_functions.c.

# 6.5.3.2 int Dam\_ge ( int id, double a, double b )

parameter derivative of c implementation of matlab function ge

### **Parameters**

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

# Returns

0

Definition at line 44 of file symbolic\_functions.c.

6.5.3.3 int am\_gt ( double a, double b )

c implementation of matlab function gt

#### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

### Returns

if(a > 0) then 1 else 0

Type: int

Definition at line 56 of file symbolic\_functions.c.

6.5.3.4 int Dam\_gt ( int id, double a, double b )

parameter derivative of c implementation of matlab function gt

### **Parameters**

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

### Returns

0

Definition at line 73 of file symbolic\_functions.c.

6.5.3.5 int am\_le ( double a, double b )

c implementation of matlab function le

#### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

# Returns

if(a  $\leq$ = 0) then 1 else 0

Type: int

Definition at line 85 of file symbolic\_functions.c.

6.5.3.6 int Dam\_le ( int id, double a, double b )

parameter derivative of c implementation of matlab function le

id	argument index for differentiation

а	value1
	Type: double
b	value2
	Type: double

#### Returns

0

Definition at line 102 of file symbolic\_functions.c.

6.5.3.7 int am\_lt ( double a, double b )

c implementation of matlab function It

### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

### Returns

if(a < 0) then 1 else 0

Type: int

Definition at line 114 of file symbolic\_functions.c.

6.5.3.8 int Dam\_It ( int id, double a, double b )

parameter derivative of c implementation of matlab function It

# **Parameters**

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

# Returns

0

Definition at line 131 of file symbolic\_functions.c.

6.5.3.9 double am\_if ( int condition, double truepart, double falsepart )

c implementation of if function

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 144 of file symbolic\_functions.c.

6.5.3.10 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 165 of file symbolic\_functions.c.

6.5.3.11 int am\_and (int a, int b)

c implementation of matlab function and

### **Parameters**

а	bool1
	Type: int
b	bool2
	Type: int

### Returns

if(a & b) then 1 else 0

Type: int

Definition at line 199 of file symbolic\_functions.c.

6.5.3.12 double Dam\_and ( int id, int a, int b )

parameter derivative of c implementation of matlab function and

### **Parameters**

id	argument index for differentiation
а	bool1
	Type: int
b	bool2
	Type: int

### Returns

0

Type: double

Definition at line 216 of file symbolic\_functions.c.

6.5.3.13 int am\_or ( int a, int b )

c implementation of matlab function or

### **Parameters**

а	bool1
	Type: int
b	bool2
	Type: int

### Returns

if(a | b) then 1 else 0

Type: int

Definition at line 228 of file symbolic\_functions.c.

6.5.3.14 double Dam\_or ( int id, int a, int b )

parameter derivative of c implementation of matlab function or

### **Parameters**

id	argument index for differentiation
а	bool1
	Type: int
b	bool2
	Type: int

# Returns

0

Type: double

Definition at line 245 of file symbolic\_functions.c.

6.5.3.15 double am\_min ( double a, double b )

c implementation of matlab function min

#### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

### Returns

if(a < b) then a else b

Type: double

Definition at line 257 of file symbolic\_functions.c.

6.5.3.16 double Dam\_min ( int id, double a, double b )

parameter derivative of c implementation of matlab function min

#### **Parameters**

id	argument index for differentiation
а	bool1
	Type: double
b	bool2
	Type: double

### Returns

id == 1: if(a < b) then 1 else 0

Type: double

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

Type: double

Definition at line 275 of file symbolic\_functions.c.

6.5.3.17 double am\_max ( double a, double b )

c implementation of matlab function min

### **Parameters**

а	value1
	Type: double
b	value2
	Type: double

# Returns

if(a > b) then a else b

Type: double

Definition at line 299 of file symbolic\_functions.c.

6.5.3.18 double Dam\_max (int id, double a, double b)

parameter derivative of c implementation of matlab function min

#### **Parameters**

id	argument index for differentiation
а	bool1
	Type: double
b	bool2
	Type: double

#### Returns

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

Type: double

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

Type: double

Definition at line 317 of file symbolic\_functions.c.

6.5.3.19 double heaviside ( double x )

c implementation of matlab function heaviside

#### **Parameters**

x argument
------------

### Returns

if(x>0) then 1 else 0

Definition at line 340 of file symbolic\_functions.c.

6.5.3.20 double dirac ( double x )

c implementation of matlab function dirac

# **Parameters**

X	argument

# Returns

if(x==0) then 1 else 0

Definition at line 355 of file symbolic\_functions.c.

6.5.3.21 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 371 of file symbolic\_functions.c.

6.5.3.22 double spline3 ( double t, double t1, double p1, double t2, double p2, double t3, double p3, int t5, double t6.5.3.22

spline function with 3 nodes

### **Parameters**

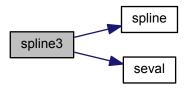
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

### Returns

spline(t)

Definition at line 395 of file symbolic\_functions.c.

Here is the call graph for this function:



6.5.3.23 double spline\_pos3 ( double t, double t,

positive spline function with 3 nodes

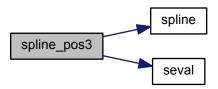
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

Returns

spline(t)

Definition at line 436 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.24 double spline4 ( double t, double t, double p, double t, dou

spline function with 4 nodes

# **Parameters**

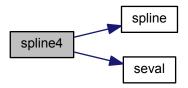
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user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

Returns

spline(t)

Definition at line 484 of file symbolic\_functions.c.

Here is the call graph for this function:



6.5.3.25 double spline\_pos4 ( double t, double t, double p, double t, double t,

positive spline function with 4 nodes

### **Parameters**

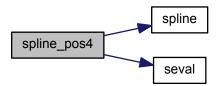
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
SS	flag indicating whether slope at first node should be user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

### Returns

spline(t)

Definition at line 528 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



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

spline function with 5 nodes

#### **Parameters**

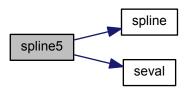
point at which the spline should be evaluated
location of node 1
spline value at node 1
location of node 2
spline value at node 2
location of node 3
spline value at node 3
location of node 4
spline value at node 4
location of node 5
spline value at node 5
flag indicating whether slope at first node should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

### Returns

spline(t)

Definition at line 580 of file symbolic\_functions.c.

Here is the call graph for this function:



6.5.3.27 double spline\_pos5 ( double t, double t1, double t2, double t2, double t3, double t3, double t4, double t5, double t5, double t5, double t6.5.3.27

positive spline function with 5 nodes

### **Parameters**

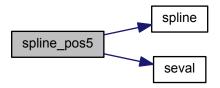
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
SS	flag indicating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

### Returns

spline(t)

Definition at line 628 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



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

spline function with 10 nodes

### **Parameters**

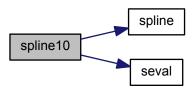
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
р3	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of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

### Returns

spline(t)

Definition at line 692 of file symbolic\_functions.c.

Here is the call graph for this function:



6.5.3.29 double spline\_pos10 ( double t, double t, double p, double t, double t

positive spline function with 10 nodes

### **Parameters**

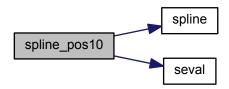
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
<i>p5</i>	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of node 8
p8	spline value at node 8
t9	location of node 9
р9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

### Returns

spline(t)

Definition at line 760 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.30 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**

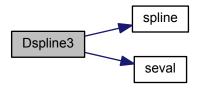
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
SS	flag indicating whether slope at first node should be user defined
dudt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

### Returns

dspline(t)dp(id)

Definition at line 821 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.31 double Dspline\_pos3 ( int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, int *ss*, double *dudt* )

parameter derivative of positive spline function with 3 nodes

### **Parameters**

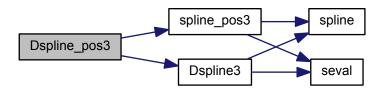
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
ss	flag indicating whether slope at first node should be user defined
dudt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

### Returns

dspline(t)dp(id)

Definition at line 866 of file symbolic\_functions.c.

Here is the call graph for this function:



6.5.3.32 double Dspline4 ( int id, double t, doub

parameter derivative of spline function with 4 nodes

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

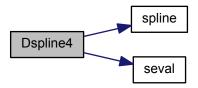
dudt	user defined slope at first node

### Returns

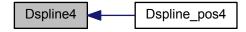
dspline(t)dp(id)

Definition at line 909 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.33 double Dspline\_pos4 ( int id, double t, double t,

parameter derivative of positive spline function with 4 nodes

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

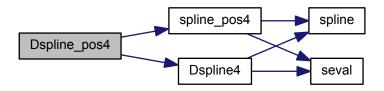
p4	spline value at node 4
ss	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

### Returns

dspline(t)dp(id)

Definition at line 958 of file symbolic\_functions.c.

Here is the call graph for this function:



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

parameter derivative of spline function with 5 nodes

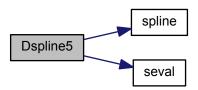
id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
p1	spline value at node 1
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5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

Returns

dspline(t)dp(id)

Definition at line 1003 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.35 double Dspline\_pos5 ( int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, int *ss*, double *dudt* )

parameter derivative of positive spline function with 5 nodes

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

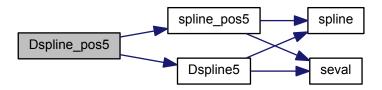
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

# Returns

dspline(t)dp(id)

Definition at line 1056 of file symbolic\_functions.c.

Here is the call graph for this function:



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

parameter derivative of spline function with 10 nodes

id	argument index for differentiation
t	point at which the spline should be evaluated
t1	location of node 1
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
<i>p5</i>	spline value at node 5
<i>t6</i>	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of node 8
p8	spline value at node 8

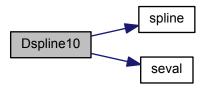
t9	location of node 9
р9	spline value at node 9
t10	location of node 10
p10	spline value at node 10
SS	flag indicating whether slope at first node should be user defined
dudt	user defined slope at first node

#### Returns

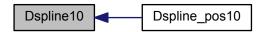
dspline(t)dp(id)

Definition at line 1112 of file symbolic\_functions.c.

Here is the call graph for this function:



Here is the caller graph for this function:



6.5.3.37 double Dspline\_pos10 ( int *id*, double *t*, double *t*1, double *p*1, double *t*2, double *p*2, double *t*3, double *p*3, double *t*4, double *p*4, double *t*5, double *p*5, double *t*6, double *p*6, double *t*7, double *p*7, double *t*8, double *p*8, double *t*9, double *p*9, double *t*10, double *p*10, int *ss*, double *dudt* )

parameter derivative of positive spline function with 10 nodes

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

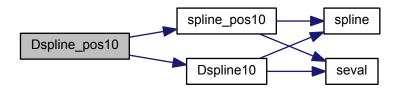
t2	location of node 2
p2	spline value at node 2
t3	location of node 3
рЗ	spline value at node 3
t4	location of node 4
p4	spline value at node 4
t5	location of node 5
p5	spline value at node 5
t6	location of node 6
p6	spline value at node 6
t7	location of node 7
p7	spline value at node 7
t8	location of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

# Returns

dspline(t)dp(id)

Definition at line 1185 of file symbolic\_functions.c.

Here is the call graph for this function:



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