

SUNDIALSB v2.4.0, a MATLAB Interface to SUNDIALS

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1 Introduction

SUNDIALS [2], SUite of Nonlinear and Differential/ALgebraic equation Solvers, is a family of software tools for integration of ODE and DAE initial value problems and for the solution of nonlinear systems of equations. It consists of CVODE, IDA, and KINSOL, and variants of these with sensitivity analysis capabilities.

SUNDIALSTB is a collection of MATLAB functions which provide interfaces to the SUNDIALS solvers.

The core of each MATLAB interface in SUNDIALSTB is a single MEX file which interfaces to the various user-callable functions for that solver. However, this MEX file should not be called directly, but rather through the user-callable functions provided for each MATLAB interface.

A major design principle for SUNDIALSTB was to provide an interface that is, as much as possible, equally familiar to both SUNDIALS users and MATLAB users. Moreover, we tried to keep the number of user-callable functions to a minimum. For example, the CVODES MATLAB interface contains only 12 such functions, 2 of which relate to forward sensitivity analysis and 4 more interface solely to the adjoint sensitivity module in CVODES. A user who is only interested in integration of ODEs and not in sensitivity analysis therefore needs to call at most 6 functions. In tune with the MATLAB ODESET function, optional solver inputs in SUNDIALSTB are specified through a single function; e.g. `CvodeSetOptions` for CVODES (a similar function is used to specify optional inputs for forward sensitivity analysis). However, unlike the ODE solvers in MATLAB, we have kept the more flexible SUNDIALS model in which a separate “solve” function (`CvodeSolve` for CVODES) must be called to return the solution at a desired output time. Solver statistics, as well as optional outputs (such as solution and solution derivatives at additional times) can be obtained at any time with calls to separate functions (`CvodeGetStats` and `CvodeGet` for CVODES).

This document provides a complete documentation for the SUNDIALSTB functions. For additional details on the methods and underlying SUNDIALS software consult also the corresponding SUNDIALS user guides [3, 4, 1].

Requirements. For parallel support, SUNDIALSTB depends on MPITB with LAM v > 7.1.1 (for MPI-2 spawning feature). The required software packages can be obtained from the following addresses.

SUNDIALS	http://www.llnl.gov/CASC/sundials
MPITB	http://atc.ugr.es/javier-bin/mpitb_eng
LAM	http://www.lam-mpi.org/

2 Installation

The following steps are required to install and setup SUNDIALSTB:

2.1 Compilation and installation of sundialsTB

As of version 2.3.0, SUNDIALSTB is distributed only with the complete SUNDIALS package.

In the sequel, we assume that the SUNDIALS package was unpacked under the directory *srcdir*. The SUNDIALSTB files are therefore in *srcdir/sundialsTB*.

Compilation and installation of the SUNDIALSTB toolbox is done by running the MATLAB script `install_STB.m` which is present in the SUNDIALSTB top directory.

1. Launch MATLAB in sundialsTB

```
% cd srcdir/sundialsTB
% matlab
```

2. Run the MATLAB script `install_STB`

Note that parallel support will be compiled into the MEX files only if `$LAMHOME` is defined and `$MPITB.ROOT` is defined and *srcdir/src/nvec_par* exists.

After the MEX files are generated, you will be asked if you wish to install the SUNDIALS_{TB} toolbox. If you answer yes, you will be then asked for the installation directory (called in the sequel *instdir*). To install SUNDIALS_{TB} for all MATLAB users (not usual), assuming MATLAB is installed under `/usr/local/matlab7`, specify *instdir* = `/usr/local/matlab7/toolbox`. To install SUNDIALS_{TB} for just one user (usual configuration), install SUNDIALS_{TB} under a directory of your choice (typically under your `matlab` working directory). In other words, specify *instdir* = `/home/user/matlab`.

2.2 Configuring Matlab's startup

After a successful installation, a SUNDIALS_{TB}.m startup script is generated in *instdir*/sundials_{TB}. This file must be called by MATLAB at initialization.

If SUNDIALS_{TB} was installed for all MATLAB users (not usual), add the SUNDIALS_{TB} startup to the system-wide startup file (by linking or copying):

```
% cd /usr/local/matlab7/toolbox/local
% ln -s ../sundialsTB/startup_STB.m .
```

and add these lines to your original local startup.m

```
% SUNDIALS Toolbox startup M-file, if it exists.
if exist('startup_STB','file')
    startup_STB
end
```

If SUNDIALS_{TB} was installed for just one user (usual configuration) and assuming you do not need to keep any previously existing startup.m, link or copy the startup_STB.m script to your working 'matlab' directory:

```
% cd ~/matlab
% ln -s sundialsTB/startup_STB.m startup.m
```

If you already have a startup.m, use the method described above, first linking (or copying) startup_STB.m to the destination subdirectory and then editing the file `/matlab/startup.m` to run startup_STB.m.

2.3 Testing the installation

If everything went fine, you should now be able to try one of the CVODES, IDAS, or KINSOL examples (in MATLAB, type 'help cvodes', 'help idas', or 'help kinsol' to see a list of all examples available). For example, go to the CVODES serial example directory:

```
% cd instdir/sundialsTB/cvode/examples_ser
```

and then launch MATLAB and execute `mcvsRoberts_dns`.

3 MATLAB Interface to CVODES

The MATLAB interface to CVODES provides access to all functionality of the CVODES solver, including IVP simulation and sensitivity analysis (both forward and adjoint).

The interface consists of several user-callable functions. In addition, the user must provide several required and optional user-supplied functions which define the problem to be solved. The user-callable functions are listed in Tables 1, 2, and 3 for IVP solution, forward sensitivity analysis (FSA), and adjoint sensitivity analysis (ASA), respectively. For completeness, some functions appear in more than one table. The types of user-supplied functions are listed in Table 4. All these functions are fully documented later in this section. For more in depth details, consult also the CVODES user guide [3].

To illustrate the use of the CVODES MATLAB interface, several example problems are provided with SUNDIALSTB, both for serial and parallel computations. Most of them are MATLAB translations of example problems provided with CVODES.

Table 1: CVODES MATLAB interface functions for ODE integration

CVodeSetOptions	create an options structure for an ODE problem.	4
CVodeQuadSetOptions	create an options structure for quadrature integration.	9
CVodeInit	allocate and initialize memory for CVODES.	11
CVodeQuadInit	allocate and initialize memory for quadrature integration.	12
CVodeReInit	reinitialize memory for CVODES.	14
CVodeQuadReInit	reinitialize memory for quadrature integration.	15
CVode	integrate the ODE problem.	17
CVodeGetStats	return statistics for the CVODES solver.	19
CVodeGet	extract data from CVODES memory.	22
CVodeFree	deallocate memory for the CVODES solver.	24
CVodeMonitor	monitoring function.	103

Table 2: CVODES MATLAB interface functions for FSA

CVodeSetOptions	create an options structure for an ODE problem.	4
CVodeQuadSetOptions	create an options structure for quadrature integration.	9
CVodeSensSetOptions	create an options structure for FSA.	10
CVodeInit	allocate and initialize memory for CVODES.	11
CVodeQuadInit	allocate and initialize memory for quadrature integration.	12
CVodeSensInit	allocate and initialize memory for FSA.	12
CVodeReInit	reinitialize memory for CVODES.	14
CVodeQuadReInit	reinitialize memory for quadrature integration.	15
CVodeSensReInit	reinitialize memory for FSA.	15
CVodeSensToggleOff	temporarily deactivates FSA.	19
CVode	integrate the ODE problem.	17
CVodeGetStats	return statistics for the CVODES solver.	19
CVodeGet	extract data from CVODES memory.	22
CVodeFree	deallocate memory for the CVODES solver.	24
CVodeMonitor	monitoring function.	103

Table 3: CVODES MATLAB interface functions for ASA

CVodeSetOptions	create an options structure for an ODE problem.	4
CVodeQuadSetOptions	create an options structure for quadrature integration.	9
CVodeInit	allocate and initialize memory for the forward problem.	11
CVodeQuadInit	allocate and initialize memory for forward quadrature integration.	12
CVodeQuadReInit	reinitialize memory for forward quadrature integration.	15
CVodeReInit	reinitialize memory for the forward problem.	14
CVodeAdjInit	allocate and initialize memory for ASA.	13
CVodeInitB	allocate and initialize a backward problem.	13
CVodeAdjReInit	reinitialize memory for ASA.	16
CVodeReInitB	reinitialize a backward problem.	16
CVode	integrate the forward ODE problem.	17
CVodeB	integrate the backward problems.	18
CVodeGetStats	return statistics for the integration of the forward problem.	19
CVodeGetStatsB	return statistics for the integration of a backward problem.	21
CVodeGet	extract data from CVODES memory.	22
CVodeFree	deallocate memory for the CVODES solver.	24
CVodeMonitor	monitoring function for forward problem.	103
CVodeMonitorB	monitoring function for backward problems.	118

3.1 Interface functions

CVodeSetOptions

PURPOSE

CVodeSetOptions creates an options structure for CVODES.

SYNOPSIS

```
function options = CVodeSetOptions(varargin)
```

DESCRIPTION

CVodeSetOptions creates an options structure for CVODES.

```
Usage: OPTIONS = CVodeSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
       OPTIONS = CVodeSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)
```

`OPTIONS = CVodeSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)` creates a CVODES options structure `OPTIONS` in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

`OPTIONS = CVodeSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)` alters an existing options structure `OLDOPTIONS`.

CVodeSetOptions with no input arguments displays all property names

Table 4: CVODES MATLAB function types

Forward problems	CVRhsFn	RHS function	25
	CVRootFn	root-finding function	26
	CVQuadRhsFn	quadrature RHS function	26
	CVSensRhsFn	sensitivity RHS function	25
	CVDenseJacFn	dense Jacobian function	27
	CVBandJacFn	banded Jacobian function	28
	CVJacTimesVecFn	Jacobian times vector function	28
	CVPrecSetupFn	preconditioner setup function	29
	CVPrecSolveFn	preconditioner solve function	30
	CVGlocalFn	RHS approximation function (BBDPre)	32
	CVGcommFn	communication function (BBDPre)	31
	CVMonitorFn	monitoring function	33
Backward problems	CVRhsFnB	RHS function	34
	CVQuadRhsFnB	quadrature RHS function	34
	CVDenseJacFnB	dense Jacobian function	35
	CVBandJacFnB	banded Jacobian function	35
	CVJacTimesVecFnB	Jacobian times vector function	36
	CVPrecSetupFnB	preconditioner setup function	37
	CVPrecSolveFnB	preconditioner solve function	38
	CVGlocalFnB	RHS approximation function (BBDPre)	39
	CVGcommFnB	communication function (BBDPre)	38
	CVMonitorFnB	monitoring function	40

and their possible values.

CVodeSetOptions properties
(See also the CVODES User Guide)

UserData - User data passed unmodified to all functions [empty]
If UserData is not empty, all user provided functions will be passed the problem data as their last input argument. For example, the RHS function must be defined as $YD = ODEFUN(T, Y, DATA)$.

LMM - Linear Multistep Method ['Adams' | 'BDF']
This property specifies whether the Adams method is to be used instead of the default Backward Differentiation Formulas (BDF) method. The Adams method is recommended for non-stiff problems, while BDF is recommended for stiff problems.

NonlinearSolver - Type of nonlinear solver used [Functional | Newton]
The 'Functional' nonlinear solver is best suited for non-stiff problems, in conjunction with the 'Adams' linear multistep method, while 'Newton' is better suited for stiff problems, using the 'BDF' method.

RelTol - Relative tolerance [positive scalar | 1e-4]
RelTol defaults to 1e-4 and is applied to all components of the solution vector. See AbsTol.

AbsTol - Absolute tolerance [positive scalar or vector | 1e-6]
The relative and absolute tolerances define a vector of error weights with components

$$ewt(i) = 1/(RelTol * |y(i)| + AbsTol) \quad \text{if AbsTol is a scalar}$$

$\text{ewt}(i) = 1/(\text{RelTol} * |y(i)| + \text{AbsTol}(i))$ if AbsTol is a vector
 This vector is used in all error and convergence tests, which use a weighted RMS norm on all error-like vectors v :
 $\text{WRMSnorm}(v) = \sqrt{(1/N) \sum_{i=1..N} (v(i) * \text{ewt}(i))^2}$,
 where N is the problem dimension.

MaxNumSteps - Maximum number of steps [positive integer | 500]
 CNode will return with an error after taking MaxNumSteps internal steps in its attempt to reach the next output time.

InitialStep - Suggested initial stepsize [positive scalar]
 By default, CNode estimates an initial stepsize h_0 at the initial time t_0 as the solution of
 $\text{WRMSnorm}(h_0^2 ydd / 2) = 1$
 where ydd is an estimated second derivative of $y(t_0)$.

MaxStep - Maximum stepsize [positive scalar | inf]
 Defines an upper bound on the integration step size.

MinStep - Minimum stepsize [positive scalar | 0.0]
 Defines a lower bound on the integration step size.

MaxOrder - Maximum method order [1-12 for Adams, 1-5 for BDF | 5]
 Defines an upper bound on the linear multistep method order.

StopTime - Stopping time [scalar]
 Defines a value for the independent variable past which the solution is not to proceed.

RootsFn - Rootfinding function [function]
 To detect events (roots of functions), set this property to the event function. See CVRootFn.

NumRoots - Number of root functions [integer | 0]
 Set NumRoots to the number of functions for which roots are monitored. If NumRoots is 0, rootfinding is disabled.

StabilityLimDet - Stability limit detection algorithm [false | true]
 Flag used to turn on or off the stability limit detection algorithm within CVODES. This property can be used only with the BDF method. In this case, if the order is 3 or greater and if the stability limit is detected, the method order is reduced.

LinearSolver - Linear solver type [Dense|Diag|Band|GMRES|BiCGStab|TFQMR]
 Specifies the type of linear solver to be used for the Newton nonlinear solver (see NonlinearSolver). Valid choices are: Dense (direct, dense Jacobian), Band (direct, banded Jacobian), Diag (direct, diagonal Jacobian), GMRES (iterative, scaled preconditioned GMRES), BiCGStab (iterative, scaled preconditioned stabilized BiCG), TFQMR (iterative, scaled transpose-free QMR). The GMRES, BiCGStab, and TFQMR are matrix-free linear solvers.

JacobianFn - Jacobian function [function]
 This property is overloaded. Set this value to a function that returns Jacobian information consistent with the linear solver used (see Linsolver). If not specified, CVODES uses difference quotient approximations. For the Dense linear solver, JacobianFn must be of type CVDenseJacFn and must return a dense Jacobian matrix. For the Band linear solver, JacobianFn must be of type CVBandJacFn and must return a banded Jacobian matrix. For the iterative linear solvers, GMRES, BiCGStab, and TFQMR, JacobianFn must be of type CVJacTimesVecFn and must return a Jacobian-vector product. This property is not used for the Diag linear solver. If these options are for a backward problem, the corresponding function types are CVDenseJacFnB for the Dense linear solver, CVBandJacFnB for the band linear solver, and CVJacTimesVecFnB for the iterative linear solvers.

KrylovMaxDim - Maximum number of Krylov subspace vectors [integer | 5]
 Specifies the maximum number of vectors in the Krylov subspace. This property is used only if an iterative linear solver, GMRES, BiCGStab, or TFQMR is used (see LinSolver).

GramSchmidtType - Gram-Schmidt orthogonalization [Classical | Modified]
 Specifies the type of Gram-Schmidt orthogonalization (classical or modified). This property is used only if the GMRES linear solver is used (see LinSolver).

PrecType - Preconditioner type [Left | Right | Both | None]
 Specifies the type of user preconditioning to be done if an iterative linear solver, GMRES, BiCGStab, or TFQMR is used (see LinSolver). PrecType must be one of the following: 'None', 'Left', 'Right', or 'Both', corresponding to no preconditioning, left preconditioning only, right preconditioning only, and both left and right preconditioning, respectively.

PrecModule - Preconditioner module [BandPre | BBDPre | UserDefined]
 If PrecModule = 'UserDefined', then the user must provide at least a preconditioner solve function (see PrecSolveFn)
 CVOIDES provides the following two general-purpose preconditioner modules:
 BandPre provide a band matrix preconditioner based on difference quotients of the ODE right-hand side function. The user must specify the lower and upper half-bandwidths through the properties LowerBwidth and UpperBwidth, respectively.
 BBDPre can be only used with parallel vectors. It provide a preconditioner matrix that is block-diagonal with banded blocks. The blocking corresponds to the distribution of the dependent variable vector y among the processors. Each preconditioner block is generated from the Jacobian of the local part (on the current processor) of a given function $g(t,y)$ approximating $f(t,y)$ (see GlocalFn). The blocks are generated by a difference quotient scheme on each processor independently. This scheme utilizes an assumed banded structure with given half-bandwidths, mldq and mudq (specified through LowerBwidthDQ and UpperBwidthDQ, respectively). However, the banded Jacobian block kept by the scheme has half-bandwidths ml and mu (specified through LowerBwidth and UpperBwidth), which may be smaller.

PrecSetupFn - Preconditioner setup function [function]
 If PrecType is not 'None', PrecSetupFn specifies an optional function which, together with PrecSolve, defines left and right preconditioner matrices (either of which can be trivial), such that the product $P_1 \cdot P_2$ is an approximation to the Newton matrix. PrecSetupFn must be of type CVPrecSetupFn or CVPrecSetupFnB for forward and backward problems, respectively.

PrecSolveFn - Preconditioner solve function [function]
 If PrecType is not 'None', PrecSolveFn specifies a required function which must solve a linear system $Pz = r$, for given r . PrecSolveFn must be of type CVPrecSolveFn or CVPrecSolveFnB for forward and backward problems, respectively.

GlocalFn - Local right-hand side approximation function for BBDPre [function]
 If PrecModule is BBDPre, GlocalFn specifies a required function that evaluates a local approximation to the ODE right-hand side. GlocalFn must be of type CVGlocalFn or CVGlocalFnB for forward and backward problems, respectively.

GcommFn - Inter-process communication function for BBDPre [function]
 If PrecModule is BBDPre, GcommFn specifies an optional function to perform any inter-process communication required for the evaluation of GlocalFn. GcommFn must be of type CVGcommFn or CVGcommFnB for forward and backward problems, respectively.

LowerBwidth - Jacobian/preconditioner lower bandwidth [integer | 0]
 This property is overloaded. If the Band linear solver is used (see LinSolver), it specifies the lower half-bandwidth of the band Jacobian approximation.

If one of the three iterative linear solvers, GMRES, BiCGStab, or TFQMR is used (see LinSolver) and if the BBDPre preconditioner module in CVODES is used (see PrecModule), it specifies the lower half-bandwidth of the retained banded approximation of the local Jacobian block. If the BandPre preconditioner module (see PrecModule) is used, it specifies the lower half-bandwidth of the band preconditioner matrix. LowerBwidth defaults to 0 (no sub-diagonals).

UpperBwidth - Jacobian/preconditioner upper bandwidth [integer | 0]
This property is overloaded. If the Band linear solver is used (see LinSolver), it specifies the upper half-bandwidth of the band Jacobian approximation. If one of the three iterative linear solvers, GMRES, BiCGStab, or TFQMR is used (see LinSolver) and if the BBDPre preconditioner module in CVODES is used (see PrecModule), it specifies the upper half-bandwidth of the retained banded approximation of the local Jacobian block. If the BandPre preconditioner module (see PrecModule) is used, it specifies the upper half-bandwidth of the band preconditioner matrix. UpperBwidth defaults to 0 (no super-diagonals).

LowerBwidthDQ - BBDPre preconditioner DQ lower bandwidth [integer | 0]
Specifies the lower half-bandwidth used in the difference-quotient Jacobian approximation for the BBDPre preconditioner (see PrecModule).

UpperBwidthDQ - BBDPre preconditioner DQ upper bandwidth [integer | 0]
Specifies the upper half-bandwidth used in the difference-quotient Jacobian approximation for the BBDPre preconditioner (see PrecModule).

MonitorFn - User-provided monitoring function [function]
Specifies a function that is called after each successful integration step. This function must have type CVMonitorFn or CVMonitorFnB, depending on whether these options are for a forward or a backward problem, respectively. Sample monitoring functions CVMonitor and CVMonitorB are provided with CVODES.

MonitorData - User-provided data for the monitoring function [struct]
Specifies a data structure that is passed to the MonitorFn function every time it is called.

SensDependent - Backward problem depending on sensitivities [false | true]
Specifies whether the backward problem right-hand side depends on forward sensitivities. If TRUE, the right-hand side function provided for this backward problem must have the appropriate type (see CVRhsFnB).

ErrorMessages - Post error/warning messages [true | false]
Note that any errors in CVodeInit will result in a Matlab error, thus stopping execution. Only subsequent calls to CVODES functions will respect the value specified for 'ErrorMessages'.

NOTES:

The properties listed above that can only be used for forward problems are: StopTime, RootsFn, and NumRoots.

The property SensDependent is relevant only for backward problems.

See also

CVodeInit, CVodeReInit, CVodeInitB, CVodeReInitB
CVRhsFn, CVRootFn,

```

CVDenseJacFn, CVBandJacFn, CVJacTimesVecFn
CVPrecSetupFn, CVPrecSolveFn
CVGlocalFn, CVGcommFn
CVMonitorFn
CVRhsFnB,
CVDenseJacFnB, CVBandJacFnB, CVJacTimesVecFnB
CVPrecSetupFnB, CVPrecSolveFnB
CVGlocalFnB, CVGcommFnB
CVMonitorFnB

```

CNodeQuadSetOptions

PURPOSE

CNodeQuadSetOptions creates an options structure for quadrature integration with CVODES.

SYNOPSIS

```
function options = CNodeQuadSetOptions(varargin)
```

DESCRIPTION

CNodeQuadSetOptions creates an options structure for quadrature integration with CVODES.

```

Usage: OPTIONS = CNodeQuadSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
       OPTIONS = CNodeQuadSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)

```

`OPTIONS = CNodeQuadSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)` creates a CVODES options structure `OPTIONS` in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

`OPTIONS = CNodeQuadSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)` alters an existing options structure `OLDOPTIONS`.

`CNodeQuadSetOptions` with no input arguments displays all property names and their possible values.

CNodeQuadSetOptions properties
(See also the CVODES User Guide)

- `ErrControl` - Error control strategy for quadrature variables [false | true]
Specifies whether quadrature variables are included in the error test.
- `RelTol` - Relative tolerance for quadrature variables [scalar 1e-4]
Specifies the relative tolerance for quadrature variables. This parameter is used only if `ErrControl` = true.
- `AbsTol` - Absolute tolerance for quadrature variables [scalar or vector 1e-6]
Specifies the absolute tolerance for quadrature variables. This parameter is used only if `ErrControl` = true.
- `SensDependent` - Backward problem depending on sensitivities [false | true]
Specifies whether the backward problem quadrature right-hand side depends on forward sensitivities. If TRUE, the right-hand side function provided for

this backward problem must have the appropriate type (see CVQuadRhsFnB).

See also

CVodeQuadInit, CVodeQuadReInit.
CVodeQuadInitB, CVodeQuadReInitB

CVodeSensSetOptions

PURPOSE

CVodeSensSetOptions creates an options structure for FSA with CVODES.

SYNOPSIS

```
function options = CVodeSensSetOptions(varargin)
```

DESCRIPTION

CVodeSensSetOptions creates an options structure for FSA with CVODES.

Usage: OPTIONS = CVodeSensSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
OPTIONS = CVodeSensSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)

OPTIONS = CVodeSensSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...) creates a CVODES options structure OPTIONS in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

OPTIONS = CVodeSensSetOptions(OLDOPTIONS,'NAME1',VALUE1,...) alters an existing options structure OLDOPTIONS.

CVodeSensSetOptions with no input arguments displays all property names and their possible values.

CVodeSensSetOptions properties
(See also the CVODES User Guide)

method - FSA solution method ['Simultaneous' | 'Staggered']

Specifies the FSA method for treating the nonlinear system solution for sensitivity variables. In the simultaneous case, the nonlinear systems for states and all sensitivities are solved simultaneously. In the staggered case, the nonlinear system for states is solved first and then the nonlinear systems for all sensitivities are solved at the same time.

ParamField - Problem parameters [string]

Specifies the name of the field in the user data structure (specified through the 'UserData' field with CVodeSetOptions) in which the nominal values of the problem parameters are stored. This property is used only if CVODES will use difference quotient approximations to the sensitivity right-hand sides (see CVSensRhsFn).

ParamList - Parameters with respect to which FSA is performed [integer vector]

Specifies a list of Ns parameters with respect to which sensitivities are to be computed. This property is used only if CVODES will use difference-quotient approximations to the sensitivity right-hand sides. Its length must be Ns,

consistent with the number of columns of `yS0` (see `CVodeSensInit`).

ParamScales - Order of magnitude for problem parameters [vector]
 Provides order of magnitude information for the parameters with respect to which sensitivities are computed. This information is used if CVODES approximates the sensitivity right-hand sides or if CVODES estimates integration tolerances for the sensitivity variables (see `RelTol` and `AbsTol`).

RelTol - Relative tolerance for sensitivity variables [positive scalar]
 Specifies the scalar relative tolerance for the sensitivity variables.
 See also `AbsTol`.

AbsTol - Absolute tolerance for sensitivity variables [row-vector or matrix]
 Specifies the absolute tolerance for sensitivity variables. `AbsTol` must be either a row vector of dimension `Ns`, in which case each of its components is used as a scalar absolute tolerance for the corresponding sensitivity vector, or a `N x Ns` matrix, in which case each of its columns is used as a vector of absolute tolerances for the corresponding sensitivity vector.
 By default, CVODES estimates the integration tolerances for sensitivity variables, based on those for the states and on the order of magnitude information for the problem parameters specified through `ParamScales`.

ErrControl - Error control strategy for sensitivity variables [false | true]
 Specifies whether sensitivity variables are included in the error control test.
 Note that sensitivity variables are always included in the nonlinear system convergence test.

DQtype - Type of DQ approx. of the sensi. RHS [Centered | Forward]
 Specifies whether to use centered (second-order) or forward (first-order) difference quotient approximations of the sensitivity equation right-hand sides. This property is used only if a user-defined sensitivity right-hand side function was not provided.

DQparam - Cut-off parameter for the DQ approx. of the sensi. RHS [scalar | 0.0]
 Specifies the value which controls the selection of the difference-quotient scheme used in evaluating the sensitivity right-hand sides (switch between simultaneous or separate evaluations of the two components in the sensitivity right-hand side). The default value 0.0 indicates the use of simultaneous approximation exclusively (centered or forward, depending on the value of `DQtype`).
 For `DQparam` ≥ 1 , CVODES uses a simultaneous approximation if the estimated DQ perturbations for states and parameters are within a factor of `DQparam`, and separate approximations otherwise. Note that a value `DQparam` < 1 will inhibit switching! This property is used only if a user-defined sensitivity right-hand side function was not provided.

See also

`CVodeSensInit`, `CVodeSensReInit`

CVodeInit

PURPOSE

`CVodeInit` allocates and initializes memory for CVODES.

SYNOPSIS

```
function status = CVodeInit(fct, lmm, nls, t0, y0, options)
```

DESCRIPTION

CVodeInit allocates and initializes memory for CVODES.

Usage: CVodeInit (ODEFUN, LMM, NLS, TO, YO [, OPTIONS])

ODEFUN is a function defining the ODE right-hand side: $y' = f(t,y)$.
This function must return a vector containing the current value of the right-hand side.
LMM is the Linear Multistep Method ('Adams' or 'BDF')
NLS is the type of nonlinear solver used ('Functional' or 'Newton')
TO is the initial value of t.
YO is the initial condition vector $y(t_0)$.
OPTIONS is an (optional) set of integration options, created with the CVodeSetOptions function.

See also: CVodeSetOptions, CVRhsFn

NOTES:

- 1) The 'Functional' nonlinear solver is best suited for non-stiff problems, in conjunction with the 'Adams' linear multistep method, while 'Newton' is better suited for stiff problems, using the 'BDF' method.
- 2) When using the 'Newton' nonlinear solver, a linear solver is also required. The default one is 'Dense', indicating the use of direct dense linear algebra (LU factorization). A different linear solver can be specified through the option 'LinearSolver' to CVodeSetOptions.

CVodeQuadInit

PURPOSE

CVodeQuadInit allocates and initializes memory for quadrature integration.

SYNOPSIS

function status = CVodeQuadInit(fctQ, yQ0, options)

DESCRIPTION

CVodeQuadInit allocates and initializes memory for quadrature integration.

Usage: CVodeQuadInit (QFUN, YQ0 [, OPTIONS])

QFUN is a function defining the right-hand sides of the quadrature ODEs $y_Q' = f_Q(t,y)$.
YQ0 is the initial conditions vector $y_Q(t_0)$.
OPTIONS is an (optional) set of QUAD options, created with the CVodeSetQuadOptions function.

See also: CVodeSetQuadOptions, CVQuadRhsFn

CVodeSensInit

PURPOSE

CVodeSensInit allocates and initializes memory for FSA with CVODES.

SYNOPSIS

```
function status = CVodeSensInit(Ns,fctS,yS0,options)
```

DESCRIPTION

CVodeSensInit allocates and initializes memory for FSA with CVODES.

Usage: CVodeSensInit (NS, SFUN, YSO [, OPTIONS])

NS is the number of parameters with respect to which sensitivities are desired

SFUN is a function defining the right-hand sides of the sensitivity ODEs $yS' = fS(t,y,yS)$.

YSO Initial conditions for sensitivity variables.
YSO must be a matrix with N rows and Ns columns, where N is the problem dimension and Ns the number of sensitivity systems.

OPTIONS is an (optional) set of FSA options, created with the CVodeSetFSAOptions function.

See also CVodeSensSetOptions, CVodeInit, CVSensRhsFn

CVodeAdjInit

PURPOSE

CVodeAdjInit allocates and initializes memory for ASA with CVODES.

SYNOPSIS

```
function status = CVodeAdjInit(steps, interp)
```

DESCRIPTION

CVodeAdjInit allocates and initializes memory for ASA with CVODES.

Usage: CVodeAdjInit(STEPS, INTEPR)

STEPS specifies the (maximum) number of integration steps between two consecutive check points.

INTERP Specifies the type of interpolation used for estimating the forward solution during the backward integration phase. INTERP should be 'Hermite', indicating cubic Hermite interpolation, or 'Polynomial', indicating variable order polynomial interpolation.

CVodeInitB

PURPOSE

CVodeInitB allocates and initializes backward memory for CVODES.

SYNOPSIS

```
function [idxB, status] = CVodeInitB(fctB, lmmB, nlsB, tB0, yB0, optionsB)
```

DESCRIPTION

CVodeInitB allocates and initializes backward memory for CVODES.

Usage: IDXB = CVodeInitB (FCTB, LMMB, NLSB, TBO, YBO [, OPTIONS])

FCTB is a function defining the adjoint ODE right-hand side.
 This function must return a vector containing the current
 value of the adjoint ODE right-hand side.
LMMB is the Linear Multistep Method ('Adams' or 'BDF')
NLSB is the type of nonlinear solver used ('Functional' or 'Newton')
TBO is the final value of t.
YBO is the final condition vector yB(tBO).
OPTIONS is an (optional) set of integration options, created with
 the CVodeSetOptions function.

CVodeInitB returns the index IDXB associated with this backward
problem. This index must be passed as an argument to any subsequent
functions related to this backward problem.

See also: CVodeSetOptions, CVodeInit, CVRhsFnB

CVodeQuadInitB

PURPOSE

CVodeQuadInitB allocates and initializes memory for backward quadrature integration.

SYNOPSIS

function status = CVodeQuadInitB(idxB, fctQB, yQB0, optionsB)

DESCRIPTION

CVodeQuadInitB allocates and initializes memory for backward quadrature integration.

Usage: CVodeQuadInitB (IDXB, QBFUN, YQB0 [, OPTIONS])

IDXB is the index of the backward problem, returned by
 CVodeInitB.
QBFUN is a function defining the right-hand sides of the
 backward ODEs $y_{QB}' = f_{QB}(t, y, y_B)$.
YQB0 is the final conditions vector yQB(tBO).
OPTIONS is an (optional) set of QUAD options, created with
 the CVodeSetQuadOptions function.

See also: CVodeInitB, CVodeSetQuadOptions, CVQuadRhsFnB

CVodeReInit

PURPOSE

CVodeReInit reinitializes memory for CVODES

SYNOPSIS

function status = CVodeReInit(t0, y0, options)

DESCRIPTION

CVodeReInit reinitializes memory for CVODES

where a prior call to CVodeInit has been made with the same problem size N . CVodeReInit performs the same input checking and initializations that CVodeInit does, but it does no memory allocation, assuming that the existing internal memory is sufficient for the new problem.

Usage: CVodeReInit (T0, Y0 [, OPTIONS])

T0 is the initial value of t .

Y0 is the initial condition vector $y(t_0)$.

OPTIONS is an (optional) set of integration options, created with the CVodeSetOptions function.

See also: CVodeSetOptions, CVodeInit

CVodeQuadReInit

PURPOSE

CVodeQuadReInit reinitializes CVODES's quadrature-related memory

SYNOPSIS

function status = CVodeQuadReInit(yQ0, options)

DESCRIPTION

CVodeQuadReInit reinitializes CVODES's quadrature-related memory assuming it has already been allocated in prior calls to CVodeInit and CVodeQuadInit.

Usage: CVodeQuadReInit (YQ0 [, OPTIONS])

YQ0 Initial conditions for quadrature variables $y_Q(t_0)$.

OPTIONS is an (optional) set of QUAD options, created with the CVodeSetQuadOptions function.

See also: CVodeSetQuadOptions, CVodeQuadInit

CVodeSensReInit

PURPOSE

CVodeSensReInit reinitializes CVODES's FSA-related memory

SYNOPSIS

function status = CVodeSensReInit(yS0, options)

DESCRIPTION

CVodeSensReInit reinitializes CVODES's FSA-related memory assuming it has already been allocated in prior calls to CVodeInit and CVodeSensInit. The number of sensitivities Ns is assumed to be unchanged since the previous call to CVodeSensInit.

Usage: CVodeSensReInit (YSO [, OPTIONS])

YSO Initial conditions for sensitivity variables.
YSO must be a matrix with N rows and Ns columns, where N is the problem dimension and Ns the number of sensitivity systems.
OPTIONS is an (optional) set of FSA options, created with the CVodeSensSetOptions function.

See also: CVodeSensSetOptions, CVodeReInit, CVodeSensInit

CVodeAdjReInit

PURPOSE

CVodeAdjReInit re-initializes memory for ASA with CVODES.

SYNOPSIS

function status = CVodeAdjReInit()

DESCRIPTION

CVodeAdjReInit re-initializes memory for ASA with CVODES.

Usage: CVodeAdjReInit

CVodeReInitB

PURPOSE

CVodeReInitB re-initializes backward memory for CVODES.

SYNOPSIS

function status = CVodeReInitB(idxB, tB0, yB0, optionsB)

DESCRIPTION

CVodeReInitB re-initializes backward memory for CVODES. where a prior call to CVodeInitB has been made with the same problem size NB. CVodeReInitB performs the same input checking and initializations that CVodeInitB does, but it does no memory allocation, assuming that the existing internal memory is sufficient for the new problem.

Usage: CVodeReInitB (IDXB, TB0, YB0 [, OPTIONSXB])

IDXB is the index of the backward problem, returned by

CVodeInitB.
 TB0 is the final value of t.
 YB0 is the final condition vector yB(tB0).
 OPTIONSB is an (optional) set of integration options, created with
 the CVodeSetOptions function.

See also: CVodeSetOptions, CVodeInitB

CVodeQuadReInitB

PURPOSE

CVodeQuadReInitB reinitializes memory for backward quadrature integration.

SYNOPSIS

```
function status = CVodeQuadReInitB(idxB, yQB0, optionsB)
```

DESCRIPTION

CVodeQuadReInitB reinitializes memory for backward quadrature integration.

Usage: CVodeQuadReInitB (IDXB, YSO [, OPTIONS])

IDXB is the index of the backward problem, returned by
 CVodeInitB.
 YQB0 is the final conditions vector yQB(tB0).
 OPTIONS is an (optional) set of QUAD options, created with
 the CVodeSetQuadOptions function.

See also: CVodeSetQuadOptions, CVodeReInitB, CVodeQuadInitB

CVode

PURPOSE

CVode integrates the ODE.

SYNOPSIS

```
function [varargout] = CVode(tout, itask)
```

DESCRIPTION

CVode integrates the ODE.

Usage: [STATUS, T, Y] = CVode (TOUT, ITASK)
 [STATUS, T, Y, YS] = CVode (TOUT, ITASK)
 [STATUS, T, Y, YQ] = CVode (TOUT, ITASK)
 [STATUS, T, Y, YQ, YS] = CVode (TOUT, ITASK)

If ITASK is 'Normal', then the solver integrates from its current internal
 T value to a point at or beyond TOUT, then interpolates to T = TOUT and returns
 Y(TOUT). If ITASK is 'OneStep', then the solver takes one internal time step

and returns in Y the solution at the new internal time. In this case, TOUT is used only during the first call to CNode to determine the direction of integration and the rough scale of the problem. In either case, the time reached by the solver is returned in T.

If quadratures were computed (see CNodeQuadInit), CNode will return their values at T in the vector YQ.

If sensitivity calculations were enabled (see CNodeSensInit), CNode will return their values at T in the matrix YS. Each row in the matrix YS represents the sensitivity vector with respect to one of the problem parameters.

In ITASK = 'Normal' mode, to obtain solutions at specific times T0,T1,...,TFINAL (all increasing or all decreasing) use TOUT = [T0 T1 ... TFINAL]. In this case the output arguments Y and YQ are matrices, each column representing the solution vector at the corresponding time returned in the vector T. If computed, the sensitivities are returned in the 3-dimensional array YS, with YS(:, :, I) representing the sensitivity vectors at the time T(I).

On return, STATUS is one of the following:

- 0: successful CNode return.
- 1: CNode succeeded and returned at tstop.
- 2: CNode succeeded and found one or more roots.

See also CNodeSetOptions, CNodeGetStats

CNodeB

PURPOSE

CNodeB integrates all backwards ODEs currently defined.

SYNOPSIS

```
function [varargout] = CNodeB(tout,itask)
```

DESCRIPTION

CNodeB integrates all backwards ODEs currently defined.

Usage: [STATUS, T, YB] = CNodeB (TOUT, ITASK)
 [STATUS, T, YB, YQB] = CNodeB (TOUT, ITASK)

If ITASK is 'Normal', then the solver integrates from its current internal T value to a point at or beyond TOUT, then interpolates to T = TOUT and returns YB(TOUT). If ITASK is 'OneStep', then the solver takes one internal time step and returns in YB the solution at the new internal time. In this case, TOUT is used only during the first call to CNodeB to determine the direction of integration and the rough scale of the problem. In either case, the time reached by the solver is returned in T.

If quadratures were computed (see CNodeQuadInitB), CNodeB will return their values at T in the vector YQB.

In ITASK = ' Normal' mode, to obtain solutions at specific times T0,T1,...,TFINAL (all increasing or all decreasing) use TOUT = [T0 T1 ... TFINAL]. In this case the output arguments YB and YQB are matrices, each column representing the solution vector at the corresponding time returned in the vector T.

If more than one backward problem was defined, the return arguments are cell arrays, with TIDXB, YBIDXB, and YQBIDXB corresponding to the backward problem with index IDXB (as returned by CNodeInitB).

On return, STATUS is one of the following:

- 0: successful CNodeB return.
- 1: CNodeB succeeded and return at a tstop value (internally set).

See also CNodeSetOptions, CNodeGetStatsB

CNodeSensToggleOff

PURPOSE

CNodeSensToggleOff deactivates sensitivity calculations.

SYNOPSIS

```
function status = CNodeSensToggleOff()
```

DESCRIPTION

CNodeSensToggleOff deactivates sensitivity calculations.

It does NOT deallocate sensitivity-related memory so that sensitivity computations can be later toggled ON (through CNodeSensReInit).

Usage: CNodeSensToggleOff

See also: CNodeSensInit, CNodeSensReInit

CNodeGetStats

PURPOSE

CNodeGetStats returns run statistics for the CVODES solver.

SYNOPSIS

```
function [si, status] = CNodeGetStats()
```

DESCRIPTION

CNodeGetStats returns run statistics for the CVODES solver.

Usage: STATS = CNodeGetStats

Fields in the structure STATS

- o nst - number of integration steps
- o nfe - number of right-hand side function evaluations
- o nsetups - number of linear solver setup calls
- o netf - number of error test failures
- o nni - number of nonlinear solver iterations
- o ncfn - number of convergence test failures
- o qlast - last method order used
- o qcur - current method order
- o h0used - actual initial step size used
- o hlast - last step size used
- o hcur - current step size
- o tcur - current time reached by the integrator
- o RootInfo - structure with rootfinding information
- o QuadInfo - structure with quadrature integration statistics
- o LSInfo - structure with linear solver statistics
- o FSAInfo - structure with forward sensitivity solver statistics

If rootfinding was requested, the structure RootInfo has the following fields

- o nge - number of calls to the rootfinding function
- o roots - array of integers (a value of 1 in the i-th component means that the i-th rootfinding function has a root (upon a return with status=2 from CVode)).

If quadratures were present, the structure QuadInfo has the following fields

- o nfQe - number of quadrature integrand function evaluations
- o netfQ - number of error test failures for quadrature variables

The structure LSInfo has different fields, depending on the linear solver used.

Fields in LSInfo for the 'Dense' linear solver

- o name - 'Dense'
- o njeD - number of Jacobian evaluations
- o nfeD - number of right-hand side function evaluations for difference-quotient Jacobian approximation

Fields in LSInfo for the 'Diag' linear solver

- o name - 'Diag'
- o nfeDI - number of right-hand side function evaluations for difference-quotient Jacobian approximation

Fields in LSInfo for the 'Band' linear solver

- o name - 'Band'
- o njeB - number of Jacobian evaluations
- o nfeB - number of right-hand side function evaluations for difference-quotient Jacobian approximation

Fields in LSInfo for the 'GMRES' and 'BiCGStab' linear solvers

- o name - 'GMRES' or 'BiCGStab'
- o nli - number of linear solver iterations
- o npe - number of preconditioner setups
- o nps - number of preconditioner solve function calls
- o ncfl - number of linear system convergence test failures
- o njeSG - number of Jacobian-vector product evaluations
- o nfeSG - number of right-hand side function evaluations for difference-quotient Jacobian-vector product approximation

If forward sensitivities were computed, the structure FSAInfo has the following fields

- o nfSe - number of sensitivity right-hand side evaluations
- o nfeS - number of right-hand side evaluations for difference-quotient sensitivity right-hand side approximation
- o nsetupS - number of linear solver setups triggered by sensitivity variables
- o netfS - number of error test failures for sensitivity variables
- o nniS - number of nonlinear solver iterations for sensitivity variables
- o ncfnS - number of convergence test failures due to sensitivity variables

CNodeGetStatsB

PURPOSE

CNodeGetStatsB returns run statistics for the backward CVODES solver.

SYNOPSIS

```
function [si, status] = CNodeGetStatsB(idxB)
```

DESCRIPTION

CNodeGetStatsB returns run statistics for the backward CVODES solver.

Usage: STATS = CNodeGetStatsB(IDXB)

IDXB is the index of the backward problem, returned by CNodeInitB.

Fields in the structure STATS

- o nst - number of integration steps
- o nfe - number of right-hand side function evaluations
- o nsetupS - number of linear solver setup calls
- o netf - number of error test failures
- o nni - number of nonlinear solver iterations
- o ncfn - number of convergence test failures
- o qlast - last method order used
- o qcur - current method order
- o h0used - actual initial step size used
- o hlast - last step size used
- o hcur - current step size
- o tcur - current time reached by the integrator
- o QuadInfo - structure with quadrature integration statistics

- o LSInfo - structure with linear solver statistics

The structure LSInfo has different fields, depending on the linear solver used.

If quadratures were present, the structure QuadInfo has the following fields

- o nfQe - number of quadrature integrand function evaluations
- o netfQ - number of error test failures for quadrature variables

Fields in LSInfo for the 'Dense' linear solver

- o name - 'Dense'
- o njeD - number of Jacobian evaluations
- o nfeD - number of right-hand side function evaluations for difference-quotient
Jacobian approximation

Fields in LSInfo for the 'Diag' linear solver

- o name - 'Diag'
- o nfeDI - number of right-hand side function evaluations for difference-quotient
Jacobian approximation

Fields in LSInfo for the 'Band' linear solver

- o name - 'Band'
- o njeB - number of Jacobian evaluations
- o nfeB - number of right-hand side function evaluations for difference-quotient
Jacobian approximation

Fields in LSInfo for the 'GMRES' and 'BiCGStab' linear solvers

- o name - 'GMRES' or 'BiCGStab'
- o nli - number of linear solver iterations
- o npe - number of preconditioner setups
- o nps - number of preconditioner solve function calls
- o ncfl - number of linear system convergence test failures
- o njeSG - number of Jacobian-vector product evaluations
- o nfeSG - number of right-hand side function evaluations for difference-quotient
Jacobian-vector product approximation

CVodeGet

PURPOSE

CVodeGet extracts data from the CVODES solver memory.

SYNOPSIS

```
function [output, status] = CVodeGet(key, varargin)
```

DESCRIPTION

CVodeGet extracts data from the CVODES solver memory.

Usage: RET = CNodeGet (KEY [, P1 [, P2] ...])

CNodeGet returns internal CNODES information based on KEY. For some values of KEY, additional arguments may be required and/or more than one output is returned.

KEY is a string and should be one of:

- o DerivSolution - Returns a vector containing the K-th order derivative of the solution at time T. The time T and order K must be passed through the input arguments P1 and P2, respectively:
DKY = CNodeGet('DerivSolution', T, K)
- o ErrorWeights - Returns a vector containing the current error weights.
EWT = CNodeGet('ErrorWeights')
- o CheckPointsInfo - Returns an array of structures with check point information.
CK = CNodeGet('CheckPointInfo')

CNodeSet

PURPOSE

CNodeSet changes optional input values during the integration.

SYNOPSIS

function status = CNodeSet(varargin)

DESCRIPTION

CNodeSet changes optional input values during the integration.

Usage: CNodeSet('NAME1',VALUE1,'NAME2',VALUE2,...)

CNodeSet can be used to change some of the optional inputs during the integration, i.e., without need for a solver reinitialization. The property names accepted by CNodeSet are a subset of those valid for CNodeSetOptions. Any unspecified properties are left unchanged.

CNodeSet with no input arguments displays all property names.

CNodeSet properties

(See also the CNODES User Guide)

UserData - problem data passed unmodified to all user functions.

Set VALUE to be the new user data.

RelTol - Relative tolerance

Set VALUE to the new relative tolerance

AbsTol - absolute tolerance

Set VALUE to be either the new scalar absolute tolerance or a vector of absolute tolerances, one for each solution component.

StopTime - Stopping time

Set VALUE to be a new value for the independent variable past which the solution is not to proceed.

CVodeSetB

PURPOSE

CVodeSetB changes optional input values during the integration.

SYNOPSIS

```
function status = CVodeSetB(idxB, varargin)
```

DESCRIPTION

CVodeSetB changes optional input values during the integration.

Usage: CVodeSetB(IDXB, 'NAME1',VALUE1,'NAME2',VALUE2,...)

CVodeSetB can be used to change some of the optional inputs for the backward problem identified by IDXB during the backward integration, i.e., without need for a solver reinitialization. The property names accepted by CVodeSet are a subset of those valid for CVodeSetOptions. Any unspecified properties are left unchanged.

CVodeSetB with no input arguments displays all property names.

CVodeSetB properties

(See also the CVODES User Guide)

UserData - problem data passed unmodified to all user functions.

Set VALUE to be the new user data.

RelTol - Relative tolerance

Set VALUE to the new relative tolerance

AbsTol - absolute tolerance

Set VALUE to be either the new scalar absolute tolerance or a vector of absolute tolerances, one for each solution component.

CVodeFree

PURPOSE

CVodeFree deallocates memory for the CVODES solver.

SYNOPSIS

```
function CVodeFree()
```

DESCRIPTION

CVodeFree deallocates memory for the CVODES solver.

Usage: CVodeFree

3.2 Function types

CVRhsFn

PURPOSE

CVRhsFn - type for user provided RHS function

SYNOPSIS

This is a script file.

DESCRIPTION

CVRhsFn - type for user provided RHS function

The function ODEFUN must be defined as

```
FUNCTION [YD, FLAG] = ODEFUN(T,Y)
```

and must return a vector YD corresponding to $f(t,y)$.

If a user data structure DATA was specified in CVodeMalloc, then

ODEFUN must be defined as

```
FUNCTION [YD, FLAG, NEW_DATA] = ODEFUN(T,Y,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector YD, the ODEFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function ODEFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVodeInit

CVSensRhsFn

PURPOSE

CVSensRhsFn - type for user provided sensitivity RHS function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVSensRhsFn - type for user provided sensitivity RHS function.

The function ODESFUN must be defined as

```
FUNCTION [YSD, FLAG] = ODESFUN(T,Y,YD,YS)
```

and must return a matrix YSD corresponding to $fS(t,y,yS)$.

If a user data structure DATA was specified in CVodeMalloc, then

ODESFUN must be defined as

```
FUNCTION [YSD, FLAG, NEW_DATA] = ODESFUN(T,Y,YD,YS,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix YSD, the ODESFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function ODESFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVodeSetFSAOptions

NOTE: ODESFUN is specified through the property FSARhsFn to CVodeSetFSAOptions.

CVQuadRhsFn

PURPOSE

CVQuadRhsFn - type for user provided quadrature RHS function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVQuadRhsFn - type for user provided quadrature RHS function.

The function ODEQFUN must be defined as

FUNCTION [YQD, FLAG] = ODEQFUN(T,Y)

and must return a vector YQD corresponding to fQ(t,y), the integrand for the integral to be evaluated.

If a user data structure DATA was specified in CVodeMalloc, then ODEQFUN must be defined as

FUNCTION [YQD, FLAG, NEW_DATA] = ODEQFUN(T,Y,DATA)

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector YQD, the ODEQFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function ODEQFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVodeQuadInit

CVRootFn

PURPOSE

CVRootFn - type for user provided root-finding function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVRootFn - type for user provided root-finding function.

The function ROOTFUN must be defined as

```
FUNCTION [G, FLAG] = ROOTFUN(T,Y)
```

and must return a vector G corresponding to $g(t,y)$.

If a user data structure DATA was specified in CVodeMalloc, then ROOTFUN must be defined as

```
FUNCTION [G, FLAG, NEW_DATA] = ROOTFUN(T,Y,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector G, the ROOTFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function ROOTFUN must set FLAG=0 if successful, or FLAG~=0 if a failure occurred.

See also CVodeSetOptions

NOTE: ROOTFUN is specified through the RootsFn property in CVodeSetOptions and is used only if the property NumRoots is a positive integer.

CVDenseJacFn

PURPOSE

CVDenseJacFn - type for user provided dense Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVDenseJacFn - type for user provided dense Jacobian function.

The function DJACFUN must be defined as

```
FUNCTION [J, FLAG] = DJACFUN(T, Y, FY)
```

and must return a matrix J corresponding to the Jacobian of $f(t,y)$.

The input argument FY contains the current value of $f(t,y)$.

If a user data structure DATA was specified in CVodeMalloc, then DJACFUN must be defined as

```
FUNCTION [J, FLAG, NEW_DATA] = DJACFUN(T, Y, FY, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J, the DJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function DJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVodeSetOptions

NOTE: DJACFUN is specified through the property JacobianFn to CNodeSetOptions and is used only if the property LinearSolver was set to 'Dense'.

CVBandJacFn

PURPOSE

CVBandJacFn - type for user provided banded Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVBandJacFn - type for user provided banded Jacobian function.

The function BJACFUN must be defined as

FUNCTION [J, FLAG] = BJACFUN(T, Y, FY)

and must return a matrix J corresponding to the banded Jacobian of f(t,y).

The input argument FY contains the current value of f(t,y).

If a user data structure DATA was specified in CNodeMalloc, then BJACFUN must be defined as

FUNCTION [J, FLAG, NEW_DATA] = BJACFUN(T, Y, FY, DATA)

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J, the BJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function BJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CNodeSetOptions

See the CNODES user guide for more information on the structure of a banded Jacobian.

NOTE: BJACFUN is specified through the property JacobianFn to CNodeSetOptions and is used only if the property LinearSolver was set to 'Band'.

CVJacTimesVecFn

PURPOSE

CVJacTimesVecFn - type for user provided Jacobian times vector function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVJacTimesVecFn - type for user provided Jacobian times vector function.

The function JTVFUN must be defined as

```
FUNCTION [JV, FLAG] = JTVFUN(T,Y,FY,V)
```

and must return a vector JV corresponding to the product of the Jacobian of $f(t,y)$ with the vector v .

The input argument FY contains the current value of $f(t,y)$.

If a user data structure DATA was specified in CVodeMalloc, then JTVFUN must be defined as

```
FUNCTION [JV, FLAG, NEW_DATA] = JTVFUN(T,Y,FY,V,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector JV, the JTVFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function JTVFUN must set FLAG=0 if successful, or FLAG~=0 if a failure occurred.

See also CVodeSetOptions

NOTE: JTVFUN is specified through the property JacobianFn to CVodeSetOptions and is used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

CVPrecSetupFn

PURPOSE

CVPrecSetupFn - type for user provided preconditioner setup function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVPrecSetupFn - type for user provided preconditioner setup function.

The user-supplied preconditioner setup function PSETFUN and the user-supplied preconditioner solve function PSOLFUN together must define left and right preconditioner matrices P1 and P2 (either of which may be trivial), such that the product $P1 \cdot P2$ is an approximation to the Newton matrix $M = I - \gamma J$. Here J is the system Jacobian $J = df/dy$, and γ is a scalar proportional to the integration step size h . The solution of systems $Pz = r$, with $P = P1$ or $P2$, is to be carried out by the PrecSolve function, and PSETFUN is to do any necessary setup operations.

The user-supplied preconditioner setup function PSETFUN is to evaluate and preprocess any Jacobian-related data needed by the preconditioner solve function PSOLFUN. This might include forming a crude approximate Jacobian,

and performing an LU factorization on the resulting approximation to M . This function will not be called in advance of every call to PSOLFUN, but instead will be called only as often as necessary to achieve convergence within the Newton iteration. If the PSOLFUN function needs no preparation, the PSETFUN function need not be provided.

For greater efficiency, the PSETFUN function may save Jacobian-related data and reuse it, rather than generating it from scratch. In this case, it should use the input flag JOK to decide whether to recompute the data, and set the output flag JCUR accordingly.

Each call to the PSETFUN function is preceded by a call to ODEFUN with the same (t,y) arguments. Thus the PSETFUN function can use any auxiliary data that is computed and saved by the ODEFUN function and made accessible to PSETFUN.

The function PSETFUN must be defined as

```
FUNCTION [JCUR, FLAG] = PSETFUN(T,Y,FY,JOK,GAMMA)
```

and must return a logical flag JCUR (true if Jacobian information was recomputed and false if saved data was reused). If PSETFUN was successful, it must return FLAG=0. For a recoverable error (in which case the setup will be retried) it must set FLAG to a positive integer value. If an unrecoverable error occurs, it must set FLAG to a negative value, in which case the integration will be halted. The input argument FY contains the current value of $f(t,y)$. If the input logical flag JOK is false, it means that Jacobian-related data must be recomputed from scratch. If it is true, it means that Jacobian data, if saved from the previous PSETFUN call can be reused (with the current value of GAMMA).

If a user data structure DATA was specified in CVodeMalloc, then PSETFUN must be defined as

```
FUNCTION [JCUR, FLAG, NEW_DATA] = PSETFUN(T,Y,FY,JOK,GAMMA,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the flags JCUR and FLAG, the PSETFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

See also CVPrecSolveFn, CVodeSetOptions

NOTE: PSETFUN is specified through the property PrecSetupFn to CVodeSetOptions and is used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR' and if the property PrecType is not 'None'.

CVPrecSolveFn

PURPOSE

CVPrecSolveFn - type for user provided preconditioner solve function.

SYNOPSIS

This is a script file.

DESCRIPTION

CVPrecSolveFn - type for user provided preconditioner solve function.

The user-supplied preconditioner solve function PSOLFVN is to solve a linear system $Pz = r$ in which the matrix P is one of the preconditioner matrices $P1$ or $P2$, depending on the type of preconditioning chosen.

The function PSOLFVN must be defined as

```
FUNCTION [Z, FLAG] = PSOLFVN(T,Y,FY,R)
```

and must return a vector Z containing the solution of $Pz=r$.

If PSOLFVN was successful, it must return $FLAG=0$. For a recoverable error (in which case the step will be retried) it must set $FLAG$ to a positive value. If an unrecoverable error occurs, it must set $FLAG$ to a negative value, in which case the integration will be halted. The input argument FY contains the current value of $f(t,y)$.

If a user data structure $DATA$ was specified in $CVodeMalloc$, then PSOLFVN must be defined as

```
FUNCTION [Z, FLAG, NEW_DATA] = PSOLFVN(T,Y,FY,R,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector Z and the flag $FLAG$, the PSOLFVN function must also set NEW_DATA . Otherwise, it should set $NEW_DATA=[]$ (do not set $NEW_DATA = DATA$ as it would lead to unnecessary copying).

See also $CVPrecSetupFn$, $CVodeSetOptions$

NOTE: PSOLFVN is specified through the property $PrecSolveFn$ to $CVodeSetOptions$ and is used only if the property $LinearSolver$ was set to 'GMRES', 'BiCGStab', or 'TFQMR' and if the property $PrecType$ is not 'None'.

CVGcommFn

PURPOSE

CVGcommFn - type for user provided communication function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

CVGcommFn - type for user provided communication function (BBDPre).

The function GCOMFUN must be defined as

```
FUNCTION FLAG = GCOMFUN(T, Y)
```

and can be used to perform all interprocess communication necessary to evaluate the approximate right-hand side function for the BBDPre preconditioner module.

If a user data structure DATA was specified in CNodeMalloc, then GCOMFUN must be defined as

```
FUNCTION [FLAG, NEW_DATA] = GCOMFUN(T, Y, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then the GCOMFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function GCOMFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVGlocalFn, CNodeSetOptions

NOTES:

GCOMFUN is specified through the GcommFn property in CNodeSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

Each call to GCOMFUN is preceded by a call to the RHS function ODEFUN with the same arguments T and Y. Thus GCOMFUN can omit any communication done by ODEFUN if relevant to the evaluation of G by GLOCFUN. If all necessary communication was done by ODEFUN, GCOMFUN need not be provided.

CVGlocalFn

PURPOSE

CVGlocalFn - type for user provided RHS approximation function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

CVGlocalFn - type for user provided RHS approximation function (BBDPre).

The function GLOCFUN must be defined as

```
FUNCTION [GLOC, FLAG] = GLOCFUN(T,Y)
```

and must return a vector GLOC corresponding to an approximation to f(t,y) which will be used in the BBDPRE preconditioner module. The case where G is mathematically identical to F is allowed.

If a user data structure DATA was specified in CNodeMalloc, then GLOCFUN must be defined as

```
FUNCTION [GLOC, FLAG, NEW_DATA] = GLOCFUN(T,Y,DATA)
```

If the local modifications to the user data structure are needed

in other user-provided functions then, besides setting the vector G, the GLOCFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function GLOCFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVGcommFn, CNodeSetOptions

NOTE: GLOCFUN is specified through the GlocalFn property in CNodeSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

CVMonitorFn

PURPOSE

CVMonitorFn - type for user provided monitoring function for forward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVMonitorFn - type for user provided monitoring function for forward problems.

The function MONFUN must be defined as

```
FUNCTION [] = MONFUN(CALL, T, Y, YQ, YS)
```

It is called after every internal CNode step and can be used to monitor the progress of the solver. MONFUN is called with CALL=0 from CNodeInit at which time it should initialize itself and it is called with CALL=2 from CNodeFree. Otherwise, CALL=1.

It receives as arguments the current time T, solution vector Y, and, if they were computed, quadrature vector YQ, and forward sensitivity matrix YS. If YQ and/or YS were not computed they are empty here.

If additional data is needed inside MONFUN, it must be defined as

```
FUNCTION NEW_MONDATA = MONFUN(CALL, T, Y, YQ, YS, MONDATA)
```

If the local modifications to the user data structure need to be saved (e.g. for future calls to MONFUN), then MONFUN must set NEW_MONDATA. Otherwise, it should set NEW_MONDATA=[] (do not set NEW_MONDATA = DATA as it would lead to unnecessary copying).

A sample monitoring function, CNodeMonitor, is provided with CNODES.

See also CNodeSetOptions, CNodeMonitor

NOTES:

MONFUN is specified through the MonitorFn property in CNodeSetOptions.
If this property is not set, or if it is empty, MONFUN is not used.
MONDATA is specified through the MonitorData property in CNodeSetOptions.

See CNodeMonitor for an implementation example.

CVRhsFnB

PURPOSE

CVRhsFnB - type for user provided RHS function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVRhsFnB - type for user provided RHS function for backward problems.

The function ODEFUNB must be defined either as

```
FUNCTION [YBD, FLAG] = ODEFUNB(T,Y,YB)
```

or as

```
FUNCTION [YBD, FLAG, NEW_DATA] = ODEFUNB(T,Y,YB,DATA)
```

depending on whether a user data structure DATA was specified in CNodeMalloc. In either case, it must return the vector YBD corresponding to $f_B(t,y,y_B)$.

The function ODEFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CNodeInitB

CVQuadRhsFnB

PURPOSE

CVQuadRhsFnB - type for user provided quadrature RHS function for backward problems

SYNOPSIS

This is a script file.

DESCRIPTION

CVQuadRhsFnB - type for user provided quadrature RHS function for backward problems

The function ODEQFUNB must be defined either as

```
FUNCTION [YQBD, FLAG] = ODEQFUNB(T,Y,YB)
```

or as

```
FUNCTION [YQBD, FLAG, NEW_DATA] = ODEQFUNB(T,Y,YB,DATA)
```

depending on whether a user data structure DATA was specified in CNodeMalloc. In either case, it must return the vector YQBD

corresponding to $f_{QB}(t,y,y_B)$, the integrand for the integral to be evaluated on the backward phase.

The function `ODEQFUNB` must set `FLAG=0` if successful, `FLAG<0` if an unrecoverable failure occurred, or `FLAG>0` if a recoverable error occurred.

See also `CVodeQuadInitB`

`CVDenseJacFnB`

PURPOSE

`CVDenseJacFnB` - type for user provided dense Jacobian function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

`CVDenseJacFnB` - type for user provided dense Jacobian function for backward problems.

The function `DJACFUNB` must be defined either as

```
FUNCTION [JB, FLAG] = DJACFUNB(T, Y, YB, FYB)
```

or as

```
FUNCTION [JB, FLAG, NEW_DATA] = DJACFUNB(T, Y, YB, FYB, DATA)
```

depending on whether a user data structure `DATA` was specified in `CVodeMalloc`. In either case, it must return the matrix `JB`, the Jacobian of $f_B(t,y,y_B)$, with respect to y_B . The input argument `FYB` contains the current value of $f(t,y,y_B)$.

The function `DJACFUNB` must set `FLAG=0` if successful, `FLAG<0` if an unrecoverable failure occurred, or `FLAG>0` if a recoverable error occurred.

See also `CVodeSetOptions`

NOTE: `DJACFUNB` is specified through the property `JacobianFn` to `CVodeSetOptions` and is used only if the property `LinearSolver` was set to 'Dense'.

`CVBandJacFnB`

PURPOSE

`CVBandJacFnB` - type for user provided banded Jacobian function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVBandJacFnB - type for user provided banded Jacobian function for backward problems.

The function BJACFUNB must be defined either as

```
FUNCTION [JB, FLAG] = BJACFUNB(T, Y, YB, FYB)
```

or as

```
FUNCTION [JB, FLAG, NEW_DATA] = BJACFUNB(T, Y, YB, FYB, DATA)
```

depending on whether a user data structure DATA was specified in CVodeMalloc. In either case, it must return the matrix JB, the Jacobian of $f(t, y, yB)$, with respect to yB . The input argument FYB contains the current value of $f(t, y, yB)$.

The function BJACFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVodeSetOptions

See the CVODES user guide for more information on the structure of a banded Jacobian.

NOTE: BJACFUNB is specified through the property JacobianFn to CVodeSetOptions and is used only if the property LinearSolver was set to 'Band'.

CVJacTimesVecFnB

PURPOSE

CVJacTimesVecFnB - type for user provided Jacobian times vector function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVJacTimesVecFnB - type for user provided Jacobian times vector function for backward problems.

The function JTVFUNB must be defined either as

```
FUNCTION [JVB, FLAG] = JTVFUNB(T, Y, YB, FYB, VB)
```

or as

```
FUNCTION [JVB, FLAG, NEW_DATA] = JTVFUNB(T, Y, YB, FYB, VB, DATA)
```

depending on whether a user data structure DATA was specified in CVodeMalloc. In either case, it must return the vector JVB, the product of the Jacobian of $f(t, y, yB)$ with respect to yB and a vector vB . The input argument FYB contains the current value of $f(t, y, yB)$.

The function JTVFUNB must set FLAG=0 if successful, or FLAG~0 if a failure occurred.

See also CVodeSetOptions

NOTE: JTVFUNB is specified through the property JacobianFn to CVodeSetOptions and is used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

CVPrecSetupFnB

PURPOSE

CVPrecSetupFnB - type for user provided preconditioner setup function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVPrecSetupFnB - type for user provided preconditioner setup function for backward problems.

The user-supplied preconditioner setup function PSETFUN and the user-supplied preconditioner solve function PSOLFUN together must define left and right preconditioner matrices P1 and P2 (either of which may be trivial), such that the product $P1 \cdot P2$ is an approximation to the Newton matrix $M = I - \gamma J$. Here J is the system Jacobian $J = df/dy$, and γ is a scalar proportional to the integration step size h. The solution of systems $P z = r$, with $P = P1$ or $P2$, is to be carried out by the PrecSolve function, and PSETFUN is to do any necessary setup operations.

The user-supplied preconditioner setup function PSETFUN is to evaluate and preprocess any Jacobian-related data needed by the preconditioner solve function PSOLFUN. This might include forming a crude approximate Jacobian, and performing an LU factorization on the resulting approximation to M. This function will not be called in advance of every call to PSOLFUN, but instead will be called only as often as necessary to achieve convergence within the Newton iteration. If the PSOLFUN function needs no preparation, the PSETFUN function need not be provided.

For greater efficiency, the PSETFUN function may save Jacobian-related data and reuse it, rather than generating it from scratch. In this case, it should use the input flag JOK to decide whether to recompute the data, and set the output flag JCUR accordingly.

Each call to the PSETFUN function is preceded by a call to ODEFUN with the same (t,y) arguments. Thus the PSETFUN function can use any auxiliary data that is computed and saved by the ODEFUN function and made accessible to PSETFUN.

The function PSETFUNB must be defined either as

```
FUNCTION [JCURB, FLAG] = PSETFUNB(T,Y,YB,FYB,JOK,GAMMAB)
```

or as

```
FUNCTION [JCURB, FLAG, NEW_DATA] = PSETFUNB(T,Y,YB,FYB,JOK,GAMMAB,DATA)
```

depending on whether a user data structure DATA was specified in CVodeMalloc. In either case, it must return the flags JCURB and FLAG.

See also `CVPrecSolveFnB`, `CVodeSetOptions`

NOTE: `PSETFUNB` is specified through the property `PrecSetupFn` to `CVodeSetOptions` and is used only if the property `LinearSolver` was set to `'GMRES'`, `'BiCGStab'`, or `'TFQMR'` and if the property `PrecType` is not `'None'`.

CVPrecSolveFnB

PURPOSE

`CVPrecSolveFnB` - type for user provided preconditioner solve function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

`CVPrecSolveFnB` - type for user provided preconditioner solve function for backward problems.

The user-supplied preconditioner solve function `PSOLFNB` is to solve a linear system $Pz = r$ in which the matrix P is one of the preconditioner matrices P_1 or P_2 , depending on the type of preconditioning chosen.

The function `PSOLFNB` must be defined either as

```
FUNCTION [ZB, FLAG] = PSOLFNB(T,Y,YB,FYB,RB)
```

or as

```
FUNCTION [ZB, FLAG, NEW_DATA] = PSOLFNB(T,Y,YB,FYB,RB,DATA)
```

depending on whether a user data structure `DATA` was specified in `CVodeMalloc`. In either case, it must return the vector `ZB` and the flag `FLAG`.

See also `CVPrecSetupFnB`, `CVodeSetOptions`

NOTE: `PSOLFNB` is specified through the property `PrecSolveFn` to `CVodeSetOptions` and is used only if the property `LinearSolver` was set to `'GMRES'`, `'BiCGStab'`, or `'TFQMR'` and if the property `PrecType` is not `'None'`.

CVGcommFnB

PURPOSE

`CVGcommFn` - type for user provided communication function (`BBDPre`) for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVGcommFn - type for user provided communication function (BBDPre) for backward problems.

The function GCOMFUNB must be defined either as

```
FUNCTION FLAG = GCOMFUNB(T, Y, YB)
```

or as

```
FUNCTION [FLAG, NEW_DATA] = GCOMFUNB(T, Y, YB, DATA)
```

depending on whether a user data structure DATA was specified in CNodeMalloc.

The function GCOMFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVGlocalFnB, CNodeSetOptions

NOTES:

GCOMFUNB is specified through the GcommFn property in CNodeSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

Each call to GCOMFUNB is preceded by a call to the RHS function ODEFUNB with the same arguments T, Y, and YB. Thus GCOMFUNB can omit any communication done by ODEFUNB if relevant to the evaluation of G by GLOCFUNB. If all necessary communication was done by ODEFUNB, GCOMFUNB need not be provided.

CVGlocalFnB

PURPOSE

CVGlocalFnB - type for user provided RHS approximation function (BBDPre) for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVGlocalFnB - type for user provided RHS approximation function (BBDPre) for backward problems.

The function GLOCFUNB must be defined either as

```
FUNCTION [GLOCB, FLAG] = GLOCFUNB(T,Y,YB)
```

or as

```
FUNCTION [GLOCB, FLAG, NEW_DATA] = GLOCFUNB(T,Y,YB,DATA)
```

depending on whether a user data structure DATA was specified in CNodeMalloc. In either case, it must return the vector GLOCB corresponding to an approximation to fB(t,y,yB).

The function GLOCFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also CVGcommFnB, CNodeSetOptions

NOTE: GLOCFUNB is specified through the GlocalFn property in CNodeSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

CVMonitorFnB

PURPOSE

CVMonitorFnB - type of user provided monitoring function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

CVMonitorFnB - type of user provided monitoring function for backward problems.

The function MONFUNB must be defined as

```
FUNCTION [] = MONFUNB(CALL, IDXB, T, Y, YQ)
```

It is called after every internal CNodeB step and can be used to monitor the progress of the solver. MONFUNB is called with CALL=0 from CNodeInitB at which time it should initialize itself and it is called with CALL=2 from CNodeFree. Otherwise, CALL=1.

It receives as arguments the index of the backward problem (as returned by CNodeInitB), the current time T, solution vector Y, and, if it was computed, the quadrature vector YQ. If quadratures were not computed for this backward problem, YQ is empty here.

If additional data is needed inside MONFUNB, it must be defined as

```
FUNCTION NEW_MONDATA = MONFUNB(CALL, IDXB, T, Y, YQ, MONDATA)
```

If the local modifications to the user data structure need to be saved (e.g. for future calls to MONFUNB), then MONFUNB must set NEW_MONDATA. Otherwise, it should set NEW_MONDATA=[] (do not set NEW_MONDATA = DATA as it would lead to unnecessary copying).

A sample monitoring function, CNodeMonitorB, is provided with CNODES.

See also CNodeSetOptions, CNodeMonitorB

NOTES:

MONFUNB is specified through the MonitorFn property in CNodeSetOptions.

If this property is not set, or if it is empty, MONFUNB is not used.

MONDATA is specified through the MonitorData property in CNodeSetOptions.

See CNodeMonitorB for an implementation example.

4 MATLAB Interface to IDAS

The MATLAB interface to IDAS provides access to all functionality of the IDAS solver, including DAE simulation and sensitivity analysis (both forward and adjoint).

The interface consists of 9 user-callable functions. The user must provide several required and optional user-supplied functions which define the problem to be solved. The user-callable functions are listed in Tables 5, 6, and 7 for IVP solution, forward sensitivity analysis (FSA), and adjoint sensitivity analysis (ASA), respectively. For completeness, some functions appear in more than one table. The types of user-supplied functions are listed in Table 8. All these functions are fully documented later in this section. For more in depth details, consult also the IDAS user guide [4].

To illustrate the use of the IDAS MATLAB interface, several example problems are provided with SUNDIALSTM, both for serial and parallel computations. Most of them are MATLAB translations of example problems provided with IDAS.

Table 5: IDAS MATLAB interface functions for DAE integration

IDASetOptions	create an options structure for an DAE problem.	42
IDAQuadSetOptions	create an options structure for quadrature integration.	46
IDAInit	allocate and initialize memory for IDAS.	49
IDAQuadInit	allocate and initialize memory for quadrature integration.	49
IDAReInit	reinitialize memory for IDAS.	52
IDAQuadReInit	reinitialize memory for quadrature integration.	52
IDACalcIC	compute consistent initial conditions.	54
IDASolve	integrate the DAE problem.	56
IDAGetStats	return statistics for the IDAS solver.	59
IDAGet	extract data from IDAS memory.	61
IDAFree	deallocate memory for the IDAS solver.	63
IDAMonitor	monitoring function.	119

Table 6: IDAS MATLAB interface functions for FSA

IDASetOptions	create an options structure for an DAE problem.	42
IDAQuadSetOptions	create an options structure for quadrature integration.	46
IDASensSetOptions	create an options structure for FSA.	47
IDAInit	allocate and initialize memory for IDAS.	49
IDAQuadInit	allocate and initialize memory for quadrature integration.	49
IDASensInit	allocate and initialize memory for FSA.	50
IDAReInit	reinitialize memory for IDAS.	52
IDAQuadReInit	reinitialize memory for quadrature integration.	52
IDASensReInit	reinitialize memory for FSA.	53
IDASensToggleOff	temporarily deactivates FSA.	58
IDACalcIC	compute consistent initial conditions.	54
IDASolve	integrate the DAE problem.	56
IDAGetStats	return statistics for the IDAS solver.	59
IDAGet	extract data from IDAS memory.	61
IDAFree	deallocate memory for the IDAS solver.	63
IDAMonitor	monitoring function.	119

Table 7: IDAS MATLAB interface functions for ASA

IDASetOptions	create an options structure for an DAE problem.	42
IDAQuadSetOptions	create an options structure for quadrature integration.	46
IDAInit	allocate and initialize memory for the forward problem.	49
IDAQuadInit	allocate and initialize memory for forward quadrature integration.	49
IDAQuadReInit	reinitialize memory for forward quadrature integration.	52
IDAREInit	reinitialize memory for the forward problem.	52
IDAAdjInit	allocate and initialize memory for ASA.	50
IDAInitB	allocate and initialize a backward problem.	51
IDAAdjReInit	reinitialize memory for ASA.	53
IDAREInitB	reinitialize a backward problem.	53
IDACalcIC	compute consistent initial conditions.	54
IDACalcICB	compute consistent initial conditions for the backward problem.	56
IDASolve	integrate the forward DAE problem.	56
IDASolveB	integrate the backward problems.	57
IDAGetStats	return statistics for the integration of the forward problem.	59
IDAGetStatsB	return statistics for the integration of a backward problem.	60
IDAGet	extract data from IDAS memory.	61
IDAFree	deallocate memory for the IDAS solver.	63
IDAMonitor	monitoring function for forward problem.	119
IDAMonitorB	monitoring function for backward problems.	134

4.1 Interface functions

IDASetOptions

PURPOSE

IDASetOptions creates an options structure for IDAS.

SYNOPSIS

```
function options = IDASetOptions(varargin)
```

DESCRIPTION

IDASetOptions creates an options structure for IDAS.

```
Usage: OPTIONS = IDASetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
       OPTIONS = IDASetOptions(OLDOPTIONS,'NAME1',VALUE1,...)
```

`OPTIONS = IDASetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)` creates a IDAS options structure `OPTIONS` in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

`OPTIONS = IDASetOptions(OLDOPTIONS,'NAME1',VALUE1,...)` alters an existing options structure `OLDOPTIONS`.

Table 8: IDAS MATLAB function types

Forward problems	IDARhsFn	residual function	64
	IDARootFn	root-finding function	65
	IDAQuadRhsFn	quadrature RHS function	65
	IDASensRhsFn	sensitivity RHS function	64
	IDADenseJacFn	dense Jacobian function	66
	IDABandJacFn	banded Jacobian function	67
	IDAJacTimesVecFn	Jacobian times vector function	67
	IDAPrecSetupFn	preconditioner setup function	68
	IDAPrecSolveFn	preconditioner solve function	69
	IDAGlocalFn	residual approximation function (BBDPRe)	71
	IDAGcommFn	communication function (BBDPRe)	70
	IDAMonitorFn	monitoring function	72
Backward problems	IDARhsFnB	residual function	73
	IDAQuadRhsFnB	quadrature RHS function	73
	IDADenseJacFnB	dense Jacobian function	74
	IDABandJacFnB	banded Jacobian function	75
	IDAJacTimesVecFnB	Jacobian times vector function	75
	IDAPrecSetupFnB	preconditioner setup function	76
	IDAPrecSolveFnB	preconditioner solve function	76
	IDAGlocalFnB	residual approximation function (BBDPRe)	78
	IDAGcommFnB	communication function (BBDPRe)	77
	IDAMonitorFnB	monitoring function	78

IDASetOptions with no input arguments displays all property names and their possible values.

IDASetOptions properties
(See also the IDAS User Guide)

UserData - User data passed unmodified to all functions [empty]
If UserData is not empty, all user provided functions will be passed the problem data as their last input argument. For example, the RES function must be defined as $R = \text{DAEFUN}(T, YY, TP, \text{DATA})$.

RelTol - Relative tolerance [positive scalar | $1e-4$]
RelTol defaults to $1e-4$ and is applied to all components of the solution vector. See AbsTol.

AbsTol - Absolute tolerance [positive scalar or vector | $1e-6$]
The relative and absolute tolerances define a vector of error weights with components

$$\begin{aligned} \text{ewt}(i) &= 1/(\text{RelTol} * |y(i)| + \text{AbsTol}) && \text{if AbsTol is a scalar} \\ \text{ewt}(i) &= 1/(\text{RelTol} * |y(i)| + \text{AbsTol}(i)) && \text{if AbsTol is a vector} \end{aligned}$$

This vector is used in all error and convergence tests, which use a weighted RMS norm on all error-like vectors v:

$$\text{WRMSnorm}(v) = \sqrt{(1/N) \sum_{i=1..N} (v(i) * \text{ewt}(i))^2},$$

where N is the problem dimension.

MaxNumSteps - Maximum number of steps [positive integer | 500]

IDASolve will return with an error after taking MaxNumSteps internal steps in its attempt to reach the next output time.

InitialStep - Suggested initial stepsize [positive scalar]
 By default, IDASolve estimates an initial stepsize h_0 at the initial time t_0 as the solution of

$$\text{WRMSnorm}(h_0^2 ydd / 2) = 1$$
 where ydd is an estimated second derivative of $y(t_0)$.

MaxStep - Maximum stepsize [positive scalar | inf]
 Defines an upper bound on the integration step size.

MaxOrder - Maximum method order [1-5 for BDF | 5]
 Defines an upper bound on the linear multistep method order.

StopTime - Stopping time [scalar]
 Defines a value for the independent variable past which the solution is not to proceed.

RootsFn - Rootfinding function [function]
 To detect events (roots of functions), set this property to the event function. See IDARootFn.

NumRoots - Number of root functions [integer | 0]
 Set NumRoots to the number of functions for which roots are monitored.
 If NumRoots is 0, rootfinding is disabled.

SuppressAlgVars - Suppress algebraic vars. from error test [on | off]

VariableTypes - Alg./diff. variables [vector]

ConstraintTypes - Simple bound constraints [vector]

LinearSolver - Linear solver type [Dense|Band|GMRES|BiCGStab|TFQMR]
 Specifies the type of linear solver to be used for the Newton nonlinear solver. Valid choices are: Dense (direct, dense Jacobian), Band (direct, banded Jacobian), GMRES (iterative, scaled preconditioned GMRES), BiCGStab (iterative, scaled preconditioned stabilized BiCG), TFQMR (iterative, scaled transpose-free QMR).
 The GMRES, BiCGStab, and TFQMR are matrix-free linear solvers.

JacobianFn - Jacobian function [function]
 This property is overloaded. Set this value to a function that returns Jacobian information consistent with the linear solver used (see LinSolver).
 If not specified, IDAS uses difference quotient approximations.
 For the Dense linear solver, JacobianFn must be of type IDADenseJacFn and must return a dense Jacobian matrix. For the Band linear solver, JacobianFn must be of type IDABandJacFn and must return a banded Jacobian matrix.
 For the iterative linear solvers, GMRES, BiCGStab, and TFQMR, JacobianFn must be of type IDAJacTimesVecFn and must return a Jacobian-vector product.

KrylovMaxDim - Maximum number of Krylov subspace vectors [integer | 5]
 Specifies the maximum number of vectors in the Krylov subspace. This property is used only if an iterative linear solver, GMRES, BiCGStab, or TFQMR is used (see LinSolver).

GramSchmidtType - Gram-Schmidt orthogonalization [Classical | Modified]
 Specifies the type of Gram-Schmidt orthogonalization (classical or modified).
 This property is used only if the GMRES linear solver is used (see LinSolver).

PrecModule - Preconditioner module [BBDPre | UserDefined]
 If PrecModule = 'UserDefined', then the user must provide at least a preconditioner solve function (see PrecSolveFn)
 IDAS provides one general-purpose preconditioner module, BBDPre, which can be only used with parallel vectors. It provides a preconditioner matrix that is block-diagonal with banded blocks. The blocking corresponds to the distribution of the dependent variable vector y among the processors.
 Each preconditioner block is generated from the Jacobian of the local part

(on the current processor) of a given function $g(t,y,y_p)$ approximating $f(t,y,y_p)$ (see `GlocalFn`). The blocks are generated by a difference quotient scheme on each processor independently. This scheme utilizes an assumed banded structure with given half-bandwidths, `mldq` and `mudq` (specified through `LowerBwidthDQ` and `UpperBwidthDQ`, respectively). However, the banded Jacobian block kept by the scheme has half-bandwidths `ml` and `mu` (specified through `LowerBwidth` and `UpperBwidth`), which may be smaller.

PrecSetupFn - Preconditioner setup function [function]
 If `PrecType` is not 'None', `PrecSetupFn` specifies an optional function which, together with `PrecSolve`, defines the preconditioner matrix, which must be an approximation to the Newton matrix. `PrecSetupFn` must be of type `IDAPrecSetupFn`.

PrecSolveFn - Preconditioner solve function [function]
 If `PrecType` is not 'None', `PrecSolveFn` specifies a required function which must solve a linear system $Pz = r$, for given r . `PrecSolveFn` must be of type `IDAPrecSolveFn`.

GlocalFn - Local residual approximation function for `BBDPre` [function]
 If `PrecModule` is `BBDPre`, `GlocalFn` specifies a required function that evaluates a local approximation to the DAE residual. `GlocalFn` must be of type `IDAGlocalFn`.

GcommFn - Inter-process communication function for `BBDPre` [function]
 If `PrecModule` is `BBDPre`, `GcommFn` specifies an optional function to perform any inter-process communication required for the evaluation of `GlocalFn`. `GcommFn` must be of type `IDAGcommFn`.

LowerBwidth - Jacobian/preconditioner lower bandwidth [integer | 0]
 This property is overloaded. If the Band linear solver is used (see `LinSolver`), it specifies the lower half-bandwidth of the band Jacobian approximation. If one of the three iterative linear solvers, `GMRES`, `BiCGStab`, or `TFQMR` is used (see `LinSolver`) and if the `BBDPre` preconditioner module in IDAS is used (see `PrecModule`), it specifies the lower half-bandwidth of the retained banded approximation of the local Jacobian block. `LowerBwidth` defaults to 0 (no sub-diagonals).

UpperBwidth - Jacobian/preconditioner upper bandwidth [integer | 0]
 This property is overloaded. If the Band linear solver is used (see `LinSolver`), it specifies the upper half-bandwidth of the band Jacobian approximation. If one of the three iterative linear solvers, `GMRES`, `BiCGStab`, or `TFQMR` is used (see `LinSolver`) and if the `BBDPre` preconditioner module in IDAS is used (see `PrecModule`), it specifies the upper half-bandwidth of the retained banded approximation of the local Jacobian block. `UpperBwidth` defaults to 0 (no super-diagonals).

LowerBwidthDQ - `BBDPre` preconditioner DQ lower bandwidth [integer | 0]
 Specifies the lower half-bandwidth used in the difference-quotient Jacobian approximation for the `BBDPre` preconditioner (see `PrecModule`).

UpperBwidthDQ - `BBDPre` preconditioner DQ upper bandwidth [integer | 0]
 Specifies the upper half-bandwidth used in the difference-quotient Jacobian approximation for the `BBDPre` preconditioner (see `PrecModule`).

MonitorFn - User-provided monitoring function [function]
 Specifies a function that is called after each successful integration step. This function must have type `IDAMonitorFn` or `IDAMonitorFnB`, depending on whether these options are for a forward or a backward problem, respectively. Sample monitoring functions `IDAMonitor` and `IDAMonitorB` are provided with IDAS.

MonitorData - User-provided data for the monitoring function [struct]
 Specifies a data structure that is passed to the `MonitorFn` function every time

it is called.

SensDependent - Backward problem depending on sensitivities [false | true]
Specifies whether the backward problem right-hand side depends on forward sensitivities. If TRUE, the residual function provided for this backward problem must have the appropriate type (see IDAResFnB).

ErrorMessages - Post error/warning messages [true | false]
Note that any errors in IDAInit will result in a Matlab error, thus stopping execution. Only subsequent calls to IDAS functions will respect the value specified for 'ErrorMessages'.

NOTES:

The properties listed above that can only be used for forward problems are: ConstraintTypes, StopTime, RootsFn, and NumRoots.

The property SensDependent is relevant only for backward problems.

See also

IDAInit, IDAReInit, IDAInitB, IDAReInitB
IDAResFn, IDARootFn
IDADenseJacFn, IDABandJacFn, IDAJacTimesVecFn
IDAPrecSetupFn, IDAPrecSolveFn
IDAGlocalFn, IDAGcommFn
IDAMonitorFn
IDAResFnB
IDADenseJacFnB, IDABandJacFnB, IDAJacTimesVecFnB
IDAPrecSetupFnB, IDAPrecSolveFnB
IDAGlocalFnB, IDAGcommFnB
IDAMonitorFnB

IDAQuadSetOptions

PURPOSE

IDAQuadSetOptions creates an options structure for IDAS.

SYNOPSIS

```
function options = IDAQuadSetOptions(varargin)
```

DESCRIPTION

IDAQuadSetOptions creates an options structure for IDAS.

Usage: OPTIONS = IDAQuadSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
OPTIONS = IDAQuadSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)

OPTIONS = IDAQuadSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...) creates an IDAS options structure OPTIONS in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

OPTIONS = IDAQuadSetOptions(OLDOPTIONS,'NAME1',VALUE1,...) alters an existing options structure OLDOPTIONS.

IDAQuadSetOptions with no input arguments displays all property names and their possible values.

IDAQuadSetOptions properties
(See also the IDAS User Guide)

ErrControl - Error control strategy for quadrature variables [on | off]

Specifies whether quadrature variables are included in the error test.

RelTol - Relative tolerance for quadrature variables [scalar 1e-4]

Specifies the relative tolerance for quadrature variables. This parameter is used only if QuadErrCon=on.

AbsTol - Absolute tolerance for quadrature variables [scalar or vector 1e-6]

Specifies the absolute tolerance for quadrature variables. This parameter is used only if QuadErrCon=on.

SensDependent - Backward problem depending on sensitivities [false | true]

Specifies whether the backward problem quadrature right-hand side depends on forward sensitivities. If TRUE, the right-hand side function provided for this backward problem must have the appropriate type (see IDAQuadRhsFnB).

See also

IDAQuadInit, IDAQuadReInit.

IDAQuadInitB, IDAQuadReInitB

IDASensSetOptions

PURPOSE

IDASensSetOptions creates an options structure for FSA with IDAS.

SYNOPSIS

```
function options = IDASensSetOptions(varargin)
```

DESCRIPTION

IDASensSetOptions creates an options structure for FSA with IDAS.

Usage: OPTIONS = IDASensSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)
OPTIONS = IDASensSetOptions(OLDOPTIONS,'NAME1',VALUE1,...)

OPTIONS = IDASensSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...) creates a IDAS options structure OPTIONS in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

OPTIONS = IDASensSetOptions(OLDOPTIONS,'NAME1',VALUE1,...) alters an existing options structure OLDOPTIONS.

IDASensSetOptions with no input arguments displays all property names and their possible values.

IDASensSetOptions properties
(See also the IDAS User Guide)

method - FSA solution method ['Simultaneous' | 'Staggered']

Specifies the FSA method for treating the nonlinear system solution for sensitivity variables. In the simultaneous case, the nonlinear systems for states and all sensitivities are solved simultaneously. In the Staggered case, the nonlinear system for states is solved first and then the nonlinear systems for all sensitivities are solved at the same time.

ParamField - Problem parameters [string]

Specifies the name of the field in the user data structure (specified through the 'UserData' field with IDASetOptions) in which the nominal values of the problem parameters are stored. This property is used only if IDAS will use difference quotient approximations to the sensitivity residuals (see IDASensResFn).

ParamList - Parameters with respect to which FSA is performed [integer vector]

Specifies a list of N_s parameters with respect to which sensitivities are to be computed. This property is used only if IDAS will use difference-quotient approximations to the sensitivity residuals. Its length must be N_s , consistent with the number of columns of y_{SO} (see IDASensInit).

ParamScales - Order of magnitude for problem parameters [vector]

Provides order of magnitude information for the parameters with respect to which sensitivities are computed. This information is used if IDAS approximates the sensitivity residuals or if IDAS estimates integration tolerances for the sensitivity variables (see RelTol and AbsTol).

RelTol - Relative tolerance for sensitivity variables [positive scalar]

Specifies the scalar relative tolerance for the sensitivity variables. See also AbsTol.

AbsTol - Absolute tolerance for sensitivity variables [row-vector or matrix]

Specifies the absolute tolerance for sensitivity variables. AbsTol must be either a row vector of dimension N_s , in which case each of its components is used as a scalar absolute tolerance for the corresponding sensitivity vector, or a $N \times N_s$ matrix, in which case each of its columns is used as a vector of absolute tolerances for the corresponding sensitivity vector.

By default, IDAS estimates the integration tolerances for sensitivity variables, based on those for the states and on the order of magnitude information for the problem parameters specified through ParamScales.

ErrControl - Error control strategy for sensitivity variables [false | true]

Specifies whether sensitivity variables are included in the error control test. Note that sensitivity variables are always included in the nonlinear system convergence test.

DQtype - Type of DQ approx. of the sensi. RHS [Centered | Forward]

Specifies whether to use centered (second-order) or forward (first-order) difference quotient approximations of the sensitivity equation residuals. This property is used only if a user-defined sensitivity residual function was not provided.

DQparam - Cut-off parameter for the DQ approx. of the sensi. RES [scalar | 0.0]

Specifies the value which controls the selection of the difference-quotient scheme used in evaluating the sensitivity residuals (switch between simultaneous or separate evaluations of the two components in the sensitivity right-hand side). The default value 0.0 indicates the use of simultaneous approximation exclusively (centered or forward, depending on the value of DQtype).

For `DQparam >= 1`, IDAS uses a simultaneous approximation if the estimated DQ perturbations for states and parameters are within a factor of `DQparam`, and separate approximations otherwise. Note that a value `DQparam < 1` will inhibit switching! This property is used only if a user-defined sensitivity residual function was not provided.

See also
`IDASensInit`, `IDASensReInit`

IDAInit

PURPOSE

`IDAMalloc` allocates and initializes memory for IDAS.

SYNOPSIS

```
function status = IDAInit(fct,t0,yy0,yp0,options)
```

DESCRIPTION

`IDAMalloc` allocates and initializes memory for IDAS.

Usage: `IDAMalloc (DAEFUN, T0, YY0, YP0 [, OPTIONS])`

DAEFUN is a function defining the DAE residual: `f(t,yy,yp)`.
This function must return a vector containing the current value of the residual.

T0 is the initial value of `t`.

YY0 is the initial condition vector `y(t0)`.

YP0 is the initial condition vector `y'(t0)`.

OPTIONS is an (optional) set of integration options, created with the `IDASetOptions` function.

See also: `IDASetOptions`, `IDAResFn`

IDAQuadInit

PURPOSE

`IDAQuadInit` allocates and initializes memory for quadrature integration.

SYNOPSIS

```
function status = IDAQuadInit(fctQ, yQ0, options)
```

DESCRIPTION

`IDAQuadInit` allocates and initializes memory for quadrature integration.

Usage: `IDAQuadInit (QFUN, YQ0 [, OPTIONS])`

QFUN is a function defining the right-hand sides of the quadrature ODEs `yQ' = fQ(t,y)`.

YQ0 is the initial conditions vector `yQ(t0)`.

OPTIONS is an (optional) set of QUAD options, created with the `IDASetQuadOptions` function.

See also: `IDASetQuadOptions`, `IDAQuadRhsFn`

IDASensInit

PURPOSE

IDASensInit allocates and initializes memory for FSA with IDAS.

SYNOPSIS

```
function status = IDASensInit(Ns,fctS,yyS0,ypS0,options)
```

DESCRIPTION

IDASensInit allocates and initializes memory for FSA with IDAS.

Usage: IDASensInit (NS, SFUN, YYS0, YPS0 [, OPTIONS])

NS is the number of parameters with respect to which sensitivities are desired

SFUN is a function defining the residual of the sensitivity DAEs $fS(t,y,yp,yS,ypS)$.

YYS0, YPS0 Initial conditions for sensitivity variables. YYS0 and YPS0 must be matrices with N rows and Ns columns, where N is the problem dimension and Ns the number of sensitivity systems.

OPTIONS is an (optional) set of FSA options, created with the IDASetFSAOptions function.

See also IDASensSetOptions, IDAInit, IDASensResFn

IDAAdjInit

PURPOSE

IDAAdjInit allocates and initializes memory for ASA with IDAS.

SYNOPSIS

```
function status = IDAAdjInit(steps, interp)
```

DESCRIPTION

IDAAdjInit allocates and initializes memory for ASA with IDAS.

Usage: IDAAdjInit(STEPS, INTEPR)

STEPS specifies the (maximum) number of integration steps between two consecutive check points.

INTERP Specifies the type of interpolation used for estimating the forward solution during the backward integration phase. INTERP should be 'Hermite', indicating cubic Hermite interpolation, or 'Polynomial', indicating variable order polynomial interpolation.

IDAInitB

PURPOSE

IDAInitB allocates and initializes backward memory for CVODES.

SYNOPSIS

```
function [idxB, status] = IDAInitB(fctB, tB0, yyB0, ypB0, optionsB)
```

DESCRIPTION

IDAInitB allocates and initializes backward memory for CVODES.

Usage: IDXB = IDAInitB (DAEFUNB, TB0, YYB0, YPB0 [, OPTIONS])

DAEFUNB is a function defining the adjoint DAE: $F(t, y, y', y_B, y_B') = 0$
This function must return a vector containing the current
value of the adjoint DAE residual.

TB0 is the final value of t .

YYB0 is the final condition vector $y_B(tB0)$.

YPB0 is the final condition vector $y_B'(tB0)$.

OPTIONS is an (optional) set of integration options, created with
the IDASetOptions function.

IDAInitB returns the index IDXB associated with this backward
problem. This index must be passed as an argument to any subsequent
functions related to this backward problem.

See also: IDASetOptions, IDAResFnB

IDAQuadInitB

PURPOSE

IDAQuadInitB allocates and initializes memory for backward quadrature integration.

SYNOPSIS

```
function status = IDAQuadInitB(idxB, fctQB, yQB0, optionsB)
```

DESCRIPTION

IDAQuadInitB allocates and initializes memory for backward quadrature integration.

Usage: IDAQuadInitB (IDXB, QBFUN, YQB0 [, OPTIONS])

IDXB is the index of the backward problem, returned by
IDAInitB.

QBFUN is a function defining the right-hand sides of the
backward ODEs $y_{QB}' = f_{QB}(t, y, y_B)$.

YQB0 is the final conditions vector $y_{QB}(tB0)$.

OPTIONS is an (optional) set of QUAD options, created with
the IDASetQuadOptions function.

See also: IDAInitB, IDASetQuadOptions, IDAQuadRhsFnB

IDAreInit

PURPOSE

IDAreInit reinitializes memory for IDAS.

SYNOPSIS

```
function status = IDAreInit(t0,yy0,yp0,options)
```

DESCRIPTION

IDAreInit reinitializes memory for IDAS.

where a prior call to IDAInit has been made with the same problem size N . IDAreInit performs the same input checking and initializations that IDAInit does, but it does no memory allocation, assuming that the existing internal memory is sufficient for the new problem.

Usage: IDAreInit (T0, YY0, YP0 [, OPTIONS])

T0 is the initial value of t .

YY0 is the initial condition vector $y(t_0)$.

YP0 is the initial condition vector $y'(t_0)$.

OPTIONS is an (optional) set of integration options, created with the IDASetOptions function.

See also: IDASetOptions, IDAInit

IDAQuadReInit

PURPOSE

IDAQuadReInit reinitializes IDAS's quadrature-related memory

SYNOPSIS

```
function status = IDAQuadReInit(yQ0, options)
```

DESCRIPTION

IDAQuadReInit reinitializes IDAS's quadrature-related memory assuming it has already been allocated in prior calls to IDAInit and IDAQuadInit.

Usage: IDAQuadReInit (YQ0 [, OPTIONS])

YQ0 Initial conditions for quadrature variables $y_Q(t_0)$.

OPTIONS is an (optional) set of QUAD options, created with the IDASetQuadOptions function.

See also: IDASetQuadOptions, IDAQuadInit

IDASensReInit

PURPOSE

IDASensReInit reinitializes IDAS's FSA-related memory

SYNOPSIS

```
function status = IDASensReInit(yyS0,ypS0,options)
```

DESCRIPTION

IDASensReInit reinitializes IDAS's FSA-related memory assuming it has already been allocated in prior calls to IDAInit and IDASensInit.
The number of sensitivities N_s is assumed to be unchanged since the previous call to IDASensInit.

Usage: IDASensReInit (YYS0, YPS0 [, OPTIONS])

YYS0, YPS0 Initial conditions for sensitivity variables.
 YYS0 and YPS0 must be matrices with N rows and N_s columns, where N is the problem dimension and N_s the number of sensitivity systems.
OPTIONS is an (optional) set of FSA options, created with the IDASetFSAOptions function.

See also: IDASensSetOptions, IDAReInit, IDASensInit

IDAAdjReInit

PURPOSE

IDAAdjReInit re-initializes memory for ASA with CVODES.

SYNOPSIS

```
function status = IDAAdjReInit()
```

DESCRIPTION

IDAAdjReInit re-initializes memory for ASA with CVODES.

Usage: IDAAdjReInit

IDAReInitB

PURPOSE

IDAReInitB allocates and initializes backward memory for IDAS.

SYNOPSIS

```
function status = IDAReInitB(idxB,tB0,yyB0,ypB0,optionsB)
```

DESCRIPTION

IDAREInitB allocates and initializes backward memory for IDAS.
 where a prior call to IDAInitB has been made with the same
 problem size NB. IDAREInitB performs the same input checking
 and initializations that IDAInitB does, but it does no
 memory allocation, assuming that the existing internal memory
 is sufficient for the new problem.

Usage: IDAREInitB (IDXB, TBO, YYBO, YPBO [, OPTIONSB])

IDXB is the index of the backward problem, returned by
 IDAInitB.
 TBO is the final value of t.
 YYBO is the final condition vector $y_B(t_{B0})$.
 YPBO is the final condition vector $y'_B(t_{B0})$.
 OPTIONSB is an (optional) set of integration options, created with
 the IDASetOptions function.

See also: IDASetOptions, IDAInitB

IDAQuadReInitB

PURPOSE

IDAQuadReInitB reinitializes memory for backward quadrature integration.

SYNOPSIS

function status = IDAQuadReInitB(idxB, yQB0, optionsB)

DESCRIPTION

IDAQuadReInitB reinitializes memory for backward quadrature integration.

Usage: IDAQuadReInitB (IDXB, YSO [, OPTIONS])

IDXB is the index of the backward problem, returned by
 IDAInitB.
 YQB0 is the final conditions vector $y_{QB}(t_{B0})$.
 OPTIONS is an (optional) set of QUAD options, created with
 the IDASetQuadOptions function.

See also: IDASetQuadOptions, IDAREInitB, IDAQuadInitB

IDACalcIC

PURPOSE

IDACalcIC computes consistent initial conditions

SYNOPSIS

function [status, varargout] = IDACalcIC(tout,icmeth)

DESCRIPTION

IDACalcIC computes consistent initial conditions

```
Usage: STATUS = IDACalcIC ( TOUT, ICMETH )
       [STATUS, YY0, YP0] = IDACalcIC ( TOUT, ICMETH )
```

IDACalcIC corrects the guess for initial conditions passed to IDAInit or IDAREInit so that the algebraic constraints are satisfied.

The argument TOUT is the first value of t at which a solution will be requested (from IDASolve). This is needed here to determine the direction of integration and rough scale in the independent variable.

If ICMETH is 'FindAlgebraic', then IDACalcIC attempts to compute the algebraic components of y and differential components of y' , given the differential components of y .

This option requires that the vector id was set through IDASetOptions specifying the differential and algebraic components.

If ICMETH is 'FindAll', then IDACalcIC attempts to compute all components of y , given y' . In this case, id is not required.

On return, STATUS is one of the following:

SUCCESS	IDACalcIC was successful. The corrected initial value vectors are in $y0$ and $yp0$.
IDA_MEM_NULL	The argument ida_mem was NULL.
IDA_ILL_INPUT	One of the input arguments was illegal. See printed message.
IDA_LINIT_FAIL	The linear solver's init routine failed.
IDA_BAD_EWT	Some component of the error weight vector is zero (illegal), either for the input value of $y0$ or a corrected value.
IDA_RES_FAIL	The user's residual routine returned a non-recoverable error flag.
IDA_FIRST_RES_FAIL	The user's residual routine returned a recoverable error flag on the first call, but IDACalcIC was unable to recover.
IDA_LSETUP_FAIL	The linear solver's setup routine had a non-recoverable error.
IDA_LSOLVE_FAIL	The linear solver's solve routine had a non-recoverable error.
IDA_NO_RECOVERY	The user's residual routine, or the linear solver's setup or solve routine had a recoverable error, but IDACalcIC was unable to recover.
IDA_CONSTR_FAIL	IDACalcIC was unable to find a solution satisfying the inequality constraints.
IDA_LINESEARCH_FAIL	The Linesearch algorithm failed to find a solution with a step larger than $steptol$ in weighted RMS norm.
IDA_CONV_FAIL	IDACalcIC failed to get convergence of the Newton iterations.

If the output arguments YY0 and YP0 are present, they will contain the consistent initial conditions.

See also: IDASetOptions, IDAInit, IDAReInit

IDACalcICB

PURPOSE

IDACalcICB computes consistent initial conditions for the backward phase.

SYNOPSIS

```
function [status, varargout] = IDACalcICB(tout,icmeth)
```

DESCRIPTION

IDACalcICB computes consistent initial conditions for the backward phase.

```
Usage: STATUS = IDACalcICB ( TOUTB, ICMETHB )  
[STATUS, YYOB, YPOB] = IDACalcIC ( TOUTB, ICMETHB )
```

See also: IDASetOptions, IDAMallocB, IDAReInitB

IDASolve

PURPOSE

IDASolve integrates the DAE.

SYNOPSIS

```
function [varargout] = IDASolve(tout,itask)
```

DESCRIPTION

IDASolve integrates the DAE.

```
Usage: [STATUS, T, Y] = IDASolve ( TOUT, ITASK )  
[STATUS, T, Y, YQ] = IDASolve (TOUT, ITASK )  
[STATUS, T, Y, YS] = IDASolve ( TOUT, ITASK )  
[STATUS, T, Y, YQ, YS] = IDASolve ( TOUT, ITASK )
```

If ITASK is 'Normal', then the solver integrates from its current internal T value to a point at or beyond TOUT, then interpolates to T = TOUT and returns Y(TOUT). If ITASK is 'OneStep', then the solver takes one internal time step and returns in Y the solution at the new internal time. In this case, TOUT is used only during the first call to IDASolve to determine the direction of integration and the rough scale of the problem. In either case, the time reached by the solver is returned in T.

If quadratures were computed (see IDAQuadInit), IDASolve will return their values at T in the vector YQ.

If sensitivity calculations were enabled (see IDASensInit), IDASolve will return their values at T in the matrix YS. Each row in the matrix YS

represents the sensitivity vector with respect to one of the problem parameters.

In ITASK = 'Normal' mode, to obtain solutions at specific times T0,T1,...,TFINAL (all increasing or all decreasing) use TOUT = [T0 T1 ... TFINAL]. In this case the output arguments Y and YQ are matrices, each column representing the solution vector at the corresponding time returned in the vector T. If computed, the sensitivities are returned in the 3-dimensional array YS, with YS(:, :, I) representing the sensitivity vectors at the time T(I).

On return, STATUS is one of the following:

- 0: IDASolve succeeded and no roots were found.
- 1: IDASolve succeeded and returned at tstop.
- 2: IDASolve succeeded, and found one or more roots.
- 1: Illegal attempt to call before IDAMalloc
- 2: One of the inputs to IDASolve is illegal. This includes the situation when a component of the error weight vectors becomes < 0 during internal time-stepping.
- 4: The solver took mxstep internal steps but could not reach TOUT. The default value for mxstep is 500.
- 5: The solver could not satisfy the accuracy demanded by the user for some internal step.
- 6: Error test failures occurred too many times (MXNEF = 7) during one internal time step or occurred with $|h| = hmin$.
- 7: Convergence test failures occurred too many times (MXNCF = 10) during one internal time step or occurred with $|h| = hmin$.
- 9: The linear solver's setup routine failed in an unrecoverable manner.
- 10: The linear solver's solve routine failed in an unrecoverable manner.

See also IDASetOptions, IDAGetStats

IDASolveB

PURPOSE

IDASolveB integrates the backward DAE.

SYNOPSIS

```
function [varargout] = IDASolveB(tout,itask)
```

DESCRIPTION

IDASolveB integrates the backward DAE.

Usage: [STATUS, T, YB] = IDASolveB (TOUT, ITASK)
[STATUS, T, YB, YQB] = IDASolveB (TOUT, ITASK)

If ITASK is 'Normal', then the solver integrates from its current internal T value to a point at or beyond TOUT, then interpolates to T = TOUT and returns YB(TOUT). If ITASK is 'OneStep', then the solver takes one internal time step and returns in YB the solution at the new internal time. In this case, TOUT is used only during the first call to IDASolveB to determine the direction of

integration and the rough scale of the problem. In either case, the time reached by the solver is returned in T.

If quadratures were computed (see IDAQuadInitB), IDASolveB will return their values at T in the vector YQB.

In ITASK = 'Normal' mode, to obtain solutions at specific times T0, T1, ..., TFINAL (all increasing or all decreasing) use TOUT = [T0 T1 ... TFINAL]. In this case the output arguments YB and YQB are matrices, each column representing the solution vector at the corresponding time returned in the vector T.

If more than one backward problem was defined, the return arguments are cell arrays, with TIDXB, YBIDXB, and YQBIDXB corresponding to the backward problem with index IDXB (as returned by IDAInitB).

On return, STATUS is one of the following:

- 0: IDASolveB succeeded.
- 1: IDASolveB succeeded and return at a tstop value (internally set).
- 2: One of the inputs to IDASolveB is illegal.
- 4: The solver took mxstep internal steps but could not reach TOUT.
The default value for mxstep is 500.
- 5: The solver could not satisfy the accuracy demanded by the user for some internal step.
- 6: Error test failures occurred too many times (MXNEF = 7) during one internal time step or occurred with $|h| = hmin$.
- 7: Convergence test failures occurred too many times (MXNCF = 10) during one internal time step or occurred with $|h| = hmin$.
- 9: The linear solver's setup routine failed in an unrecoverable manner.
- 10: The linear solver's solve routine failed in an unrecoverable manner.
- 101: Illegal attempt to call before initializing adjoint sensitivity (see IDAInit).
- 104: Illegal attempt to call before IDAInitB.
- 108: Wrong value for TOUT.

See also IDASetOptions, IDAGetStatsB

IDASensToggleOff

PURPOSE

IDASensToggleOff deactivates sensitivity calculations.

SYNOPSIS

```
function status = IDASensToggleOff()
```

DESCRIPTION

IDASensToggleOff deactivates sensitivity calculations.

It does NOT deallocate sensitivity-related memory so that sensitivity computations can be later toggled ON (through IDASensReInit).

Usage: IDASensToggleOff

See also: IDASensInit, IDASensReInit

IDAGetStats

PURPOSE

IDAGetStats returns run statistics for the IDAS solver.

SYNOPSIS

```
function [si, status] = IDAGetStats()
```

DESCRIPTION

IDAGetStats returns run statistics for the IDAS solver.

Usage: STATS = IDAGetStats

Fields in the structure STATS

- o nst - number of integration steps
- o nre - number of residual function evaluations
- o nsetups - number of linear solver setup calls
- o netf - number of error test failures
- o nni - number of nonlinear solver iterations
- o ncfn - number of convergence test failures
- o qlast - last method order used
- o qcur - current method order
- o h0used - actual initial step size used
- o hlast - last step size used
- o hcur - current step size
- o tcur - current time reached by the integrator
- o RootInfo - structure with rootfinding information
- o QuadInfo - structure with quadrature integration statistics
- o LSInfo - structure with linear solver statistics
- o FSAInfo - structure with forward sensitivity solver statistics

If rootfinding was requested, the structure RootInfo has the following fields

- o nge - number of calls to the rootfinding function
- o roots - array of integers (a value of 1 in the i-th component means that the i-th rootfinding function has a root (upon a return with status=2 from IDASolve)).

If quadratures were present, the structure QuadInfo has the following fields

- o nfQe - number of quadrature integrand function evaluations
- o netfQ - number of error test failures for quadrature variables

The structure LSInfo has different fields, depending on the linear solver used.

Fields in LSInfo for the 'Dense' linear solver

- o name - 'Dense'
- o njeD - number of Jacobian evaluations
- o nreD - number of residual function evaluations for difference-quotient

Jacobian approximation

Fields in LSinfo for the 'Band' linear solver

- o name - 'Band'
- o njeB - number of Jacobian evaluations
- o nreB - number of residual function evaluations for difference-quotient
Jacobian approximation

Fields in LSinfo for the 'GMRES' and 'BiCGStab' linear solvers

- o name - 'GMRES' or 'BiCGStab'
- o nli - number of linear solver iterations
- o npe - number of preconditioner setups
- o nps - number of preconditioner solve function calls
- o ncfl - number of linear system convergence test failures
- o njeSG - number of Jacobian-vector product evaluations
- o nreSG - number of residual function evaluations for difference-quotient
Jacobian-vector product approximation

If forward sensitivities were computed, the structure FSAInfo has the following fields

- o nrSe - number of sensitivity residual evaluations
- o nreS - number of residual evaluations for difference-quotient
sensitivity residual approximation
- o nsetupsS - number of linear solver setups triggered by sensitivity variables
- o netfS - number of error test failures for sensitivity variables
- o nniS - number of nonlinear solver iterations for sensitivity variables
- o ncfnS - number of convergence test failures due to sensitivity variables

IDAGetStatsB

PURPOSE

IDAGetStatsB returns run statistics for the backward IDAS solver.

SYNOPSIS

```
function [si, status] = IDAGetStatsB(idxB)
```

DESCRIPTION

IDAGetStatsB returns run statistics for the backward IDAS solver.

Usage: STATS = IDAGetStatsB(IDXB)

IDXB is the index of the backward problem, returned by IDAInitB.

Fields in the structure STATS

- o nst - number of integration steps
- o nre - number of residual function evaluations
- o nsetups - number of linear solver setup calls

- o netf - number of error test failures
- o nni - number of nonlinear solver iterations
- o ncfn - number of convergence test failures
- o qlast - last method order used
- o qcur - current method order
- o h0used - actual initial step size used
- o hlast - last step size used
- o hcur - current step size
- o tcur - current time reached by the integrator
- o QuadInfo - structure with quadrature integration statistics
- o LSInfo - structure with linear solver statistics

The structure LSInfo has different fields, depending on the linear solver used.

If quadratures were present, the structure QuadInfo has the following fields

- o nfQe - number of quadrature integrand function evaluations
- o netfQ - number of error test failures for quadrature variables

Fields in LSInfo for the 'Dense' linear solver

- o name - 'Dense'
- o njeD - number of Jacobian evaluations
- o nreD - number of residual function evaluations for difference-quotient
Jacobian approximation

Fields in LSInfo for the 'Band' linear solver

- o name - 'Band'
- o njeB - number of Jacobian evaluations
- o nreB - number of residual function evaluations for difference-quotient
Jacobian approximation

Fields in LSInfo for the 'GMRES' and 'BiCGStab' linear solvers

- o name - 'GMRES' or 'BiCGStab'
- o nli - number of linear solver iterations
- o npe - number of preconditioner setups
- o nps - number of preconditioner solve function calls
- o ncfl - number of linear system convergence test failures
- o njeSG - number of Jacobian-vector product evaluations
- o nreSG - number of residual function evaluations for difference-quotient
Jacobian-vector product approximation

IDAGet

PURPOSE

IDAGet extracts data from the IDAS solver memory.

SYNOPSIS

```
function [output, status] = IDAGet(key, varargin)
```

DESCRIPTION

IDAGet extracts data from the IDAS solver memory.

Usage: RET = IDAGet (KEY [, P1 [, P2] ...])

IDAGet returns internal IDAS information based on KEY. For some values of KEY, additional arguments may be required and/or more than one output is returned.

KEY is a string and should be one of:

- o DerivSolution - Returns a vector containing the K-th order derivative of the solution at time T. The time T and order K must be passed through the input arguments P1 and P2, respectively:
DKY = IDAGet('DerivSolution', T, K)
- o ErrorWeights - Returns a vector containing the current error weights.
EWT = IDAGet('ErrorWeights')
- o CheckPointsInfo - Returns an array of structures with check point information.
CK = IDAGet('CheckPointInfo')

IDASet

PURPOSE

IDASet changes optional input values during the integration.

SYNOPSIS

function status = IDASet(varargin)

DESCRIPTION

IDASet changes optional input values during the integration.

Usage: IDASet('NAME1',VALUE1,'NAME2',VALUE2,...)

IDASet can be used to change some of the optional inputs during the integration, i.e., without need for a solver reinitialization. The property names accepted by IDASet are a subset of those valid for IDASetOptions. Any unspecified properties are left unchanged.

IDASet with no input arguments displays all property names.

IDASet properties

(See also the IDAS User Guide)

UserData - problem data passed unmodified to all user functions.

Set VALUE to be the new user data.

RelTol - Relative tolerance

Set VALUE to the new relative tolerance

AbsTol - absolute tolerance

Set VALUE to be either the new scalar absolute tolerance or a vector of absolute tolerances, one for each solution component.

StopTime - Stopping time

Set VALUE to be a new value for the independent variable past which the solution is not to proceed.

IDASetB

PURPOSE

IDASetB changes optional input values during the integration.

SYNOPSIS

```
function status = IDASetB(idxB, varargin)
```

DESCRIPTION

IDASetB changes optional input values during the integration.

Usage: IDASetB(IDXB, 'NAME1',VALUE1,'NAME2',VALUE2,...)

IDASetB can be used to change some of the optional inputs for the backward problem identified by IDXB during the backward integration, i.e., without need for a solver reinitialization. The property names accepted by IDASet are a subset of those valid for IDASetOptions. Any unspecified properties are left unchanged.

IDASetB with no input arguments displays all property names.

IDASetB properties

(See also the IDAS User Guide)

UserData - problem data passed unmodified to all user functions.

Set VALUE to be the new user data.

RelTol - Relative tolerance

Set VALUE to the new relative tolerance

AbsTol - absolute tolerance

Set VALUE to be either the new scalar absolute tolerance or a vector of absolute tolerances, one for each solution component.

IDAFree

PURPOSE

IDAFree deallocates memory for the IDAS solver.

SYNOPSIS

```
function [] = IDAFree()
```

DESCRIPTION

IDAFree deallocates memory for the IDAS solver.

Usage: IDAFree

4.2 Function types

IDAResFn

PURPOSE

IDAResFn - type for residual function

SYNOPSIS

This is a script file.

DESCRIPTION

IDAResFn - type for residual function

The function DAEFUN must be defined as

```
FUNCTION [R, FLAG] = DAEFUN(T, YY, YP)
```

and must return a vector R corresponding to $f(t, yy, yp)$.

If a user data structure DATA was specified in IDAMalloc, then

DAEFUN must be defined as

```
FUNCTION [R, FLAG, NEW_DATA] = DAEFUN(T, YY, YP, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector YD, the DAEFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function DAEFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAInit

IDASensResFn

PURPOSE

IDASensRhsFn - type for user provided sensitivity RHS function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDASensRhsFn - type for user provided sensitivity RHS function.

The function DAESFUN must be defined as

```
FUNCTION [RS, FLAG] = DAESFUN(T, YY, YP, YYS, YPS)
```

and must return a matrix RS corresponding to $fS(t, yy, yp, yyS, ypS)$.

If a user data structure DATA was specified in IDAMalloc, then

DAESFUN must be defined as

```
FUNCTION [RS, FLAG, NEW_DATA] = DAESFUN(T, YY, YP, YYS, YPS, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix YSD, the ODESFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function DAESFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDASSetFSAOptions

NOTE: DAESFUN is specified through the property FSAResFn to IDASSetFSAOptions.

IDAQuadRhsFn

PURPOSE

IDAQuadRhsFn - type for user provided quadrature RHS function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAQuadRhsFn - type for user provided quadrature RHS function.

The function QFUN must be defined as

FUNCTION [YQD, FLAG] = QFUN(T, YY, YP)

and must return a vector YQD corresponding to $f_Q(t, yy, yp)$, the integrand for the integral to be evaluated.

If a user data structure DATA was specified in IDAMalloc, then QFUN must be defined as

FUNCTION [YQD, FLAG, NEW_DATA] = QFUN(T, YY, YP, DATA)

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector YQD, the QFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function QFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAQuadInit

IDARootFn

PURPOSE

IDARootFn - type for user provided root-finding function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDARootFn - type for user provided root-finding function.

The function ROOTFUN must be defined as

```
FUNCTION [G, FLAG] = ROOTFUN(T,YY,YP)
```

and must return a vector G corresponding to $g(t,yy,yp)$.

If a user data structure DATA was specified in IDAMalloc, then

ROOTFUN must be defined as

```
FUNCTION [G, FLAG, NEW_DATA] = ROOTFUN(T,YY,YP,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector G, the ROOTFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function ROOTFUN must set FLAG=0 if successful, or FLAG~=0 if a failure occurred.

See also IDASetOptions

NOTE: ROOTFUN is specified through the RootsFn property in IDASetOptions and is used only if the property NumRoots is a positive integer.

IDADenseJacFn

PURPOSE

IDADenseJacFn - type for dense Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDADenseJacFn - type for dense Jacobian function.

The function DJACFUN must be defined as

```
FUNCTION [J, FLAG] = DJACFUN(T, YY, YP, RR, CJ)
```

and must return a matrix J corresponding to the Jacobian $(df/dyy + cj*df/dyp)$.

The input argument RR contains the current value of $f(t,yy,yp)$.

If a user data structure DATA was specified in IDAMalloc, then

DJACFUN must be defined as

```
FUNCTION [J, FLAG, NEW_DATA] = DJACFUN(T, YY, YP, RR, CJ, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J, the DJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function DJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDASetOptions

NOTE: DJACFUN is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'Dense'.

IDABandJacFn

PURPOSE

IDABandJacFn - type for banded Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDABandJacFn - type for banded Jacobian function.

The function BJACFUN must be defined as

```
FUNCTION [J, FLAG] = BJACFUN(T, YY, YP, RR, CJ)
```

and must return a matrix J corresponding to the banded Jacobian (df/dyy + cj*df/dyp).

The input argument RR contains the current value of f(t,yy,yp).

If a user data structure DATA was specified in IDAMalloc, then BJACFUN must be defined as

```
FUNCTION [J, FLAG, NEW_DATA] = BJACFUN(T, YY, YP, RR, CJ, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J, the BJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function BJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDASetOptions

See the IDAS user guide for more information on the structure of a banded Jacobian.

NOTE: BJACFUN is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'Band'.

IDAJacTimesVecFn

PURPOSE

IDAJacTimesVecFn - type for Jacobian times vector function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAJacTimesVecFn - type for Jacobian times vector function.

The function JTVFUN must be defined as

```
FUNCTION [JV, FLAG] = JTVFUN(T,YY,YP,RR,V,CJ)
```

and must return a vector JV corresponding to the product of the Jacobian ($df/dyy + cj * df/dyp$) with the vector v.

The input argument RR contains the current value of $f(t,yy,yp)$.

If a user data structure DATA was specified in IDAMalloc, then JTVFUN must be defined as

```
FUNCTION [JV, FLAG, NEW_DATA] = JTVFUN(T,YY,YP,RR,V,CJ,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector JV, the JTVFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function JTVFUN must set FLAG=0 if successful, or FLAG~=0 if a failure occurred.

See also IDASetOptions

NOTE: JTVFUN is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAPrecSetupFn

PURPOSE

IDAPrecSetupFn - type for preconditioner setup function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAPrecSetupFn - type for preconditioner setup function.

The user-supplied preconditioner setup function PSETFUN and the user-supplied preconditioner solve function PSOLFUN together must define a preconditioner matrix P which is an approximation to the Newton matrix $M = J_{yy} - cj * J_{yp}$. Here $J_{yy} = df/dyy$, $J_{yp} = df/dyp$, and cj is a scalar proportional to the integration step size h. The solution of systems $Pz = r$, is to be carried out by the PrecSolve function, and PSETFUN is to do any necessary setup operations.

The user-supplied preconditioner setup function PSETFUN is to evaluate and preprocess any Jacobian-related data needed by the preconditioner solve function PSOLFUN. This might include forming a crude approximate Jacobian, and performing an LU factorization on the resulting approximation to M. This function will not be called in

advance of every call to PSOLFUN, but instead will be called only as often as necessary to achieve convergence within the Newton iteration. If the PSOLFUN function needs no preparation, the PSETFUN function need not be provided.

For greater efficiency, the PSETFUN function may save Jacobian-related data and reuse it, rather than generating it from scratch. In this case, it should use the input flag JOK to decide whether to recompute the data, and set the output flag JCUR accordingly.

Each call to the PSETFUN function is preceded by a call to DAEFUN with the same (t,yy,yp) arguments. Thus the PSETFUN function can use any auxiliary data that is computed and saved by the DAEFUN function and made accessible to PSETFUN.

The function PSETFUN must be defined as

```
FUNCTION FLAG = PSETFUN(T,YY,YP,RR,CJ)
```

If successful, it must return FLAG=0. For a recoverable error (in which case the setup will be retried) it must set FLAG to a positive integer value. If an unrecoverable error occurs, it must set FLAG to a negative value, in which case the integration will be halted. The input argument RR contains the current value of f(t,yy,yp).

If a user data structure DATA was specified in IDAMalloc, then PSETFUN must be defined as

```
FUNCTION [FLAG,NEW_DATA] = PSETFUN(T,YY,YP,RR,CJ,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the flags JCUR and FLAG, the PSETFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

See also IDAPrecSolveFn, IDASetOptions

NOTE: PSETFUN and PSETFUNB are specified through the property PrecSetupFn to IDASetOptions and are used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAPrecSolveFn

PURPOSE

IDAPrecSolveFn - type for preconditioner solve function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAPrecSolveFn - type for preconditioner solve function.

The user-supplied preconditioner solve function PSOLFUN

is to solve a linear system $Pz = r$, where P is the preconditioner matrix.

The function PSOLFUN must be defined as

```
FUNCTION [Z, FLAG] = PSOLFUN(T,YY,YP,RR,R)
```

and must return a vector Z containing the solution of $Pz=r$.

If PSOLFUN was successful, it must return $FLAG=0$. For a recoverable error (in which case the step will be retried) it must set $FLAG$ to a positive value. If an unrecoverable error occurs, it must set $FLAG$ to a negative value, in which case the integration will be halted. The input argument RR contains the current value of $f(t,yy,yp)$.

If a user data structure $DATA$ was specified in IDAMalloc, then PSOLFUN must be defined as

```
FUNCTION [Z, FLAG, NEW_DATA] = PSOLFUN(T,YY,YP,RR,R,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector Z and the flag $FLAG$, the PSOLFUN function must also set NEW_DATA . Otherwise, it should set $NEW_DATA=[]$ (do not set $NEW_DATA = DATA$ as it would lead to unnecessary copying).

See also IDAPrecSetupFn, IDASetOptions

NOTE: PSOLFUN and PSOLFUNB are specified through the property PrecSolveFn to IDASetOptions and are used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAGcommFn

PURPOSE

IDAGcommFn - type for communication function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

IDAGcommFn - type for communication function (BBDPre).

The function GCOMFUN must be defined as

```
FUNCTION FLAG = GCOMFUN(T, YY, YP)
```

and can be used to perform all interprocess communication necessary to evaluate the approximate residual function for the BBDPre preconditioner module.

If a user data structure $DATA$ was specified in IDAMalloc, then GCOMFUN must be defined as

```
FUNCTION [FLAG, NEW_DATA] = GCOMFUN(T, YY, YP, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then the GCOMFUN function must also set NEW_DATA . Otherwise, it should set $NEW_DATA=[]$ (do not set $NEW_DATA = DATA$ as it would lead to unnecessary copying).

The function GCOMFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAGlocalFn, IDASetOptions

NOTES:

GCOMFUN is specified through the GcommFn property in IDASetOptions and is used only if the property PrecModule is set to 'BBDPre'.

Each call to GCOMFUN is preceded by a call to the residual function DAEFUN with the same arguments T, YY, and YP.

Thus GCOMFUN can omit any communication done by DAEFUN if relevant to the evaluation of G by GLOCFUN. If all necessary communication was done by DAEFUN, GCOMFUN need not be provided.

IDAGlocalFn

PURPOSE

IDAGlocalFn - type for RES approximation function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

IDAGlocalFn - type for RES approximation function (BBDPre).

The function GLOCFUN must be defined as

```
FUNCTION [GLOC, FLAG] = GLOCFUN(T,YY,YP)
```

and must return a vector GLOC corresponding to an approximation to $f(t,yy,yp)$ which will be used in the BBDPRE preconditioner module. The case where G is mathematically identical to F is allowed.

If a user data structure DATA was specified in IDAMalloc, then GLOCFUN must be defined as

```
FUNCTION [GLOC, FLAG, NEW_DATA] = GLOCFUN(T,YY,YP,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector G, the GLOCFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function GLOCFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAGcommFn, IDASetOptions

NOTE: GLOCFUN and GLOCFUNB are specified through the GlocalFn property in IDASetOptions and are used only if the property PrecModule is set to 'BBDPre'.

IDAMonitorFn

PURPOSE

IDAMonitorFn - type for monitoring function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAMonitorFn - type for monitoring function.

The function MONFUN must be defined as

```
FUNCTION [] = MONFUN(CALL, T, YY, YP, YQ, YYS, YPS)
```

To enable monitoring using a given monitor function MONFUN, use IDASetOptions to set the property 'MonitorFn' to 'MONFUN' (or to @MONFUN).

MONFUN is called with the following input arguments:

- o CALL indicates the phase during the integration process at which MONFUN is called:
 - CALL=1 : MONFUN was called at the initial time; this can be either after IDAMalloc or after IDAReInit.
(typically, MONFUN should perform its own initialization)
 - CALL=2 : MONFUN was called right before a solver reinitialization.
(typically, MONFUN should decide whether to initialize itself or else to continue monitoring)
 - CALL=3 : MONFUN was called during solver finalization.
(typically, MONFUN should finalize monitoring)
 - CALL=0 : MONFUN was called after the solver took a successful internal step.
(typically, MONFUN should collect and/or display data)
- o T is the current integration time
- o YY and YP are vectors containing the solution and solution derivative at time T
- o YQ is a vector containing the quadrature variables at time T
- o YYS and YPS are matrices containing the forward sensitivities and their derivatives, respectively, at time T.

If additional data is needed inside a MONFUN function, then it must be defined as

```
FUNCTION NEW_MONDATA = MONFUN(CALL, T, YY, YP, YQ, YYS, YPS, MONDATA)
```

In this case, the MONFUN function is passed the additional argument MONDATA, the same as that specified through the property 'MonitorData' in IDASetOptions. If the local modifications to the monitor data structure

need to be saved (e.g. for future calls to MONFUN), then MONFUN must set NEW_MONDATA. Otherwise, it should set NEW_MONDATA=[] (do not set NEW_MONDATA = DATA as it would lead to unnecessary copying).

NOTES:

1. MONFUN is specified through the MonitorFn property in IDASetOptions. If this property is not set, or if it is empty, MONFUN is not used. MONDATA is specified through the MonitorData property in IDASetOptions.
2. If quadrature integration is not enabled, YQ is empty. Similarly, if forward sensitivity analysis is not enabled, YYS and YPS are empty.
3. When CALL = 2 or 3, all arguments YY, YP, YQ, YYS, and YPS are empty. Moreover, when CALL = 3, T = 0.0
4. If MONFUN is used on the backward integration phase, YYS and YPS are always empty.

See also IDASetOptions, IDAMonitor

IDAResFnB

PURPOSE

IDAResFnB - type for residual function for backward problems

SYNOPSIS

This is a script file.

DESCRIPTION

IDAResFnB - type for residual function for backward problems

The function DAEFUNB must be defined either as

```
FUNCTION [RB, FLAG] = DAEFUNB(T, YY, YP, YYB, YPB)
```

or as

```
FUNCTION [RB, FLAG, NEW_DATA] = DAEFUNB(T, YY, YP, YYB, YPB, DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the vector RB corresponding to $fB(t, yy, yp, yyB, ypB)$.

The function DAEFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAInitB, IDARhsFn

IDAQuadRhsFnB

PURPOSE

IDAQuadRhsFnB - type for quadrature RHS function for backward problems

SYNOPSIS

This is a script file.

DESCRIPTION

IDAQuadRhsFnB - type for quadrature RHS function for backward problems

The function QFUNB must be defined either as

```
FUNCTION [YQBD, FLAG] = QFUNB(T, YY, YP, YYB, YPB)
```

or as

```
FUNCTION [YQBD, FLAG, NEW_DATA] = QFUNB(T, YY, YP, YYB, YPB, DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the vector YQBD corresponding to $f_{QB}(t, yy, yp, yyB, ypB)$, the integrand for the integral to be evaluated on the backward phase.

The function QFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAQuadInitB

IDADenseJacFnB

PURPOSE

IDADenseJacFnB - type for dense Jacobian function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDADenseJacFnB - type for dense Jacobian function for backward problems.

The function DJACFUNB must be defined either as

```
FUNCTION [JB, FLAG] = DJACFUNB(T, YY, YP, YYB, YPB, RRB, CJB)
```

or as

```
FUNCTION [JB, FLAG, NEW_DATA] = DJACFUNB(T, YY, YP, YYB, YPB, RRB, CJB, DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the matrix JB, the Jacobian ($dfB/dyyB + cjb*dfB/dypB$). The input argument RRB contains the current value of $f(t, yy, yp, yyB, ypB)$.

The function DJACFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDADenseJacFn, IDASetOptions

NOTE: DJACFUNB is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'Dense'.

IDABandJacFnB

PURPOSE

IDABandJacFnB - type for banded Jacobian function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDABandJacFnB - type for banded Jacobian function for backward problems.

The function BJACFUNB must be defined either as

```
FUNCTION [JB, FLAG] = BJACFUNB(T, YY, YP, YYB, YPB, RRB, CJB)
```

or as

```
FUNCTION [JB, FLAG, NEW_DATA] = BJACFUNB(T, YY, YP, YYB, YPB, RRB, CJB)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the matrix JB, the Jacobian ($dfB/dyyB + cJB*dfB/dypB$) of $fB(t, y, yB)$. The input argument RRB contains the current value of $f(t, yy, yp, yyB, ypB)$.

The function BJACFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDASetOptions

See the IDAS user guide for more information on the structure of a banded Jacobian.

NOTE: BJACFUNB is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'Band'.

IDAJacTimesVecFnB

PURPOSE

IDAJacTimesVecFn - type for Jacobian times vector function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAJacTimesVecFn - type for Jacobian times vector function for backward problems.

The function JTVFUNB must be defined either as

```
FUNCTION [JVB, FLAG] = JTVFUNB(T, YY, YP, YYB, YPB, RRB, VB, CJB)
```

or as

```
FUNCTION [JVB, FLAG, NEW_DATA] = JTVFUNB(T, YY, YP, YYB, YPB, RRB, VB, CJB, DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the vector JVB, the product of the Jacobian ($dfB/dyyB + c_j * dfB/dypB$) and a vector vB. The input argument RRB contains the current value of $f(t,yy,yp,yyB,ypB)$.

The function JTVFUNB must set FLAG=0 if successful, or FLAG~=0 if a failure occurred.

See also IDASetOptions

NOTE: JTVFUNB is specified through the property JacobianFn to IDASetOptions and is used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAPrecSetupFnB

PURPOSE

IDAPrecSetupFnB - type for preconditioner setup function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAPrecSetupFnB - type for preconditioner setup function for backward problems.

The function PSETFUNB must be defined either as

```
FUNCTION FLAG = PSETFUNB(T,YY,YP,YYB,YPB,RRB,CJB)
```

or as

```
FUNCTION [FLAG,NEW_DATA] = PSETFUNB(T,YY,YP,YYB,YPB,RRB,CJB,DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc.

See also IDAPrecSolveFnB, IDAPrecSetupFn, IDASetOptions

NOTE: PSETFUN and PSETFUNB are specified through the property PrecSetupFn to IDASetOptions and are used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAPrecSolveFnB

PURPOSE

IDAPrecSolveFnB - type for preconditioner solve function.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAPrecSolveFnB - type for preconditioner solve function.

The user-supplied preconditioner solve function PSOLFUNB is to solve a linear system $Pz = r$, where P is the preconditioner matrix.

The function PSOLFUNB must be defined either as

```
FUNCTION [ZB,FLAG] = PSOLFUNB(T,YY,YP,YYB,YPB,RRB,RB)
```

or as

```
FUNCTION [ZB,FLAG,NEW_DATA] = PSOLFUNB(T,YY,YP,YYB,YPB,RRB,RB,DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the vector ZB and the flag FLAG.

See also IDAPrecSetupFnB, IDAPrecSolveFn, IDASetOptions

NOTE: PSOLFUN and PSOLFUNB are specified through the property PrecSolveFn to IDASetOptions and are used only if the property LinearSolver was set to 'GMRES', 'BiCGStab', or 'TFQMR'.

IDAGcommFnB

PURPOSE

IDAGcommFnB - type for communication function (BBDPre) for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAGcommFnB - type for communication function (BBDPre) for backward problems.

The function GCOMFUNB must be defined either as

```
FUNCTION FLAG = GCOMFUNB(T, YY, YP, YYB, YPB)
```

or as

```
FUNCTION [FLAG, NEW_DATA] = GCOMFUNB(T, YY, YP, YYB, YPB, DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc.

The function GCOMFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAGlocalFnB, IDAGcommFn, IDASetOptions

NOTES:

GCOMFUNB is specified through the GcommFn property in IDASetOptions and is used only if the property PrecModule is set to 'BBDPre'.

Each call to GCOMFUNB is preceded by a call to the residual function DAEFUN with the same arguments T, YY, YP and YYB and YPB.

Thus GCOMFUNB can omit any communication done by DAEFUNB if relevant to the evaluation of G by GLOCFUNB. If all necessary communication was done by DAEFUNB, GCOMFUNB need not be provided.

IDAGlocalFnB

PURPOSE

IDAGlocalFnB - type for RES approximation function (BBDPRe) for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAGlocalFnB - type for RES approximation function (BBDPRe) for backward problems.

The function GLOCFUNB must be defined either as

```
FUNCTION [GLOCB, FLAG] = GLOCFUNB(T,YY,YP,YYB,YPB)
```

or as

```
FUNCTION [GLOCB, FLAG, NEW_DATA] = GLOCFUNB(T,YY,YP,YYB,YPB,DATA)
```

depending on whether a user data structure DATA was specified in IDAMalloc. In either case, it must return the vector GLOCB corresponding to an approximation to $fB(t,yy,yp,yyB,ypB)$.

The function GLOCFUNB must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also IDAGcommFnB, IDAGlocalFn, IDASetOptions

NOTE: GLOCFUN and GLOCFUNB are specified through the GlocalFn property in IDASetOptions and are used only if the property PrecModule is set to 'BBDPRe'.

IDAMonitorFnB

PURPOSE

IDAMonitorFnB - type of monitoring function for backward problems.

SYNOPSIS

This is a script file.

DESCRIPTION

IDAMonitorFnB - type of monitoring function for backward problems.

The function MONFUNB must be defined as

```
FUNCTION [] = MONFUNB(CALL, IDXB, T, Y, YQ)
```

It is called after every internal IDASolveB step and can be used to monitor the progress of the solver. MONFUNB is called with CALL=0 from IDAInitB at which time it should initialize itself and it is called with CALL=2 from IDAFree. Otherwise, CALL=1.

It receives as arguments the index of the backward problem (as

returned by IDAInitB), the current time T, solution vector Y, and, if it was computed, the quadrature vector YQ. If quadratures were not computed for this backward problem, YQ is empty here.

If additional data is needed inside MONFUNB, it must be defined as

```
FUNCTION NEW_MONDATA = MONFUNB(CALL, IDXB, T, Y, YQ, MONDATA)
```

If the local modifications to the user data structure need to be saved (e.g. for future calls to MONFUNB), then MONFUNB must set NEW_MONDATA. Otherwise, it should set NEW_MONDATA=[] (do not set NEW_MONDATA = DATA as it would lead to unnecessary copying).

A sample monitoring function, IDAMonitorB, is provided with CVODES.

See also IDASetOptions, IDAMonitorB

NOTES:

MONFUNB is specified through the MonitorFn property in IDASetOptions. If this property is not set, or if it is empty, MONFUNB is not used. MONDATA is specified through the MonitorData property in IDASetOptions.

See IDAMonitorB for an implementation example.

5 MATLAB Interface to KINSOL

The MATLAB interface to KINSOL provides access to all functionality of the KINSOL solver.

The interface consists of 5 user-callable functions. The user must provide several required and optional user-supplied functions which define the problem to be solved. The user-callable functions and the types of user-supplied functions are listed in Table 9 and fully documented later in this section. For more in depth details, consult also the KINSOL user guide [1].

To illustrate the use of the KINSOL MATLAB interface, several example problems are provided with SUNDIALSTB, both for serial and parallel computations. Most of them are MATLAB translations of example problems provided with KINSOL.

Table 9: KINSOL MATLAB interface functions

Functions	KINSetOptions	creates an options structure for KINSOL.
	KINInit	allocates and initializes memory for KINSOL.
	KINSol	solves the nonlinear problem.
	KINGetStats	returns statistics for the KINSOL solver.
	KINFree	deallocates memory for the KINSOL solver.
Function types	KINSysFn	system function
	KINDenseJacFn	dense Jacobian function
	KINBandJacFn	banded Jacobian function
	KINJacTimesVecFn	Jacobian times vector function
	KINPrecSetupFn	preconditioner setup function
	KINPrecSolveFn	preconditioner solve function
	KINGlocalFn	system approximation function (BBDPre)
	KINGcommFn	communication function (BBDPre)

5.1 Interface functions

KINSetOptions

PURPOSE

KINSetOptions creates an options structure for KINSOL.

SYNOPSIS

```
function options = KINSetOptions(varargin)
```

DESCRIPTION

KINSetOptions creates an options structure for KINSOL.

Usage:

`options = KINSetOptions('NAME1',VALUE1,'NAME2',VALUE2,...)` creates a KINSOL options structure `options` in which the named properties have the specified values. Any unspecified properties have default values. It is sufficient to type only the leading characters that uniquely identify the property. Case is ignored for property names.

`options = KINSetOptions(oldoptions,'NAME1',VALUE1,...)` alters an existing options structure `oldoptions`.

`options = KINSetOptions(oldoptions,newoptions)` combines an existing options structure `oldoptions` with a new options structure `newoptions`. Any new properties overwrite corresponding old properties.

KINSetOptions with no input arguments displays all property names and their possible values.

KINSetOptions properties

(See also the KINSOL User Guide)

UserData - User data passed unmodified to all functions [empty]

If **UserData** is not empty, all user provided functions will be passed the problem data as their last input argument. For example, the **SYS** function must be defined as `YD = ODEFUN(T,Y,DATA)`.

MaxNumIter - maximum number of nonlinear iterations [scalar | 200]

Specifies the maximum number of iterations that the nonlinear solver is allowed to take.

FuncRelErr - relative residual error [scalar | eps]

Specifies the relative error in computing $f(y)$ when used in difference quotient approximation of matrix-vector product $J(y)*v$.

FuncNormTol - residual stopping criteria [scalar | $\text{eps}^{(1/3)}$]

Specifies the stopping tolerance on $\|f\text{scale}*\text{ABS}(f(y))\|_{L\text{-infinity}}$

ScaledStepTol - step size stopping criteria [scalar | $\text{eps}^{(2/3)}$]

Specifies the stopping tolerance on the maximum scaled step length:
$$\| y_{(k+1)} - y_k \|$$

```

|| ----- ||_L-infinity
|| |y_(k+1)| + yscale ||
MaxNewtonStep - maximum Newton step size [ scalar | 0.0 ]
    Specifies the maximum allowable value of the scaled length of the Newton step.
InitialSetup - initial call to linear solver setup [ false | true ]
    Specifies whether or not KINSol makes an initial call to the linear solver
    setup function.
MaxNumSetups - [ scalar | 10 ]
    Specifies the maximum number of nonlinear iterations between calls to the
    linear solver setup function (i.e. Jacobian/preconditioner evaluation)
MaxNumSubSetups - [ scalar | 5 ]
    Specifies the maximum number of nonlinear iterations between checks by the
    nonlinear residual monitoring algorithm (specifies length of subintervals).
    NOTE: MaxNumSetups should be a multiple of MaxNumSubSetups.
MaxNumBetaFails - maximum number of beta-condition failures [ scalar | 10 ]
    Specifies the maximum number of beta-condition failures in the line search
    algorithm.
EtaForm - Inexact Newton method [ Constant | Type2 | Type1 ]
    Specifies the method for computing the eta coefficient used in the calculation
    of the linear solver convergence tolerance (used only if strategy='InexactNewton'
    in the call to KINSol):
        lintol = (eta + eps)*||f*scale*f(y)||_L2
    which is the used to check if the following inequality is satisfied:
        ||f*scale*(f(y)+J(y)*p)||_L2 <= lintol
    Valid choices are:
        ||f(y_(k+1))||_L2 - ||f(y_k)+J(y_k)*p_k||_L2 |
EtaForm='Type1' eta = -----
                        ||f(y_k)||_L2

                        [ ||f(y_(k+1))||_L2 ]^alpha
EtaForm='Type2' eta = gamma * [ ----- ]
                        [ ||f(y_k)||_L2 ]

EtaForm='Constant'
Eta - constant value for eta [ scalar | 0.1 ]
    Specifies the constant value for eta in the case EtaForm='Constant'.
EtaAlpha - alpha parameter for eta [ scalar | 2.0 ]
    Specifies the parameter alpha in the case EtaForm='Type2'
EtaGamma - gamma parameter for eta [ scalar | 0.9 ]
    Specifies the parameter gamma in the case EtaForm='Type2'
MinBoundEps - lower bound on eps [ false | true ]
    Specifies whether or not the value of eps is bounded below by 0.01*FuncNormtol.
Constraints - solution constraints [ vector ]
    Specifies additional constraints on the solution components.
        Constraints(i) = 0 : no constrain on y(i)
        Constraints(i) = 1 : y(i) >= 0
        Constraints(i) = -1 : y(i) <= 0
        Constraints(i) = 2 : y(i) > 0
        Constraints(i) = -2 : y(i) < 0
    If Constraints is not specified, no constraints are applied to y.

LinearSolver - Type of linear solver [ Dense | Band | GMRES | BiCGStab | TFQMR ]
    Specifies the type of linear solver to be used for the Newton nonlinear solver.
    Valid choices are: Dense (direct, dense Jacobian), GMRES (iterative, scaled
    preconditioned GMRES), BiCGStab (iterative, scaled preconditioned stabilized

```

BiCG), TFQMR (iterative, scaled preconditioned transpose-free QMR).
The GMRES, BiCGStab, and TFQMR are matrix-free linear solvers.

JacobianFn - Jacobian function [function]
This property is overloaded. Set this value to a function that returns Jacobian information consistent with the linear solver used (see `LinSolver`). If not specified, KINSOL uses difference quotient approximations. For the Dense linear solver, JacobianFn must be of type `KINDenseJacFn` and must return a dense Jacobian matrix. For the iterative linear solvers, GMRES, BiCGStab, or TFQMR, JacobianFn must be of type `KINJactimesVecFn` and must return a Jacobian-vector product.

KrylovMaxDim - Maximum number of Krylov subspace vectors [scalar | 10]
Specifies the maximum number of vectors in the Krylov subspace. This property is used only if an iterative linear solver, GMRES, BiCGStab, or TFQMR is used (see `LinSolver`).

MaxNumRestarts - Maximum number of GMRES restarts [scalar | 0]
Specifies the maximum number of times the GMRES (see `LinearSolver`) solver can be restarted.

PrecModule - Built-in preconditioner module [`BBDPre` | `UserDefined`]
If the `PrecModule` = 'UserDefined', then the user must provide at least a preconditioner solve function (see `PrecSolveFn`). KINSOL provides a built-in preconditioner module, `BBDPre` which can only be used with parallel vectors. It provide a preconditioner matrix that is block-diagonal with banded blocks. The blocking corresponds to the distribution of the variable vector among the processors. Each preconditioner block is generated from the Jacobian of the local part (on the current processor) of a given function $g(t,y)$ approximating $f(y)$ (see `GlocalFn`). The blocks are generated by a difference quotient scheme on each processor independently. This scheme utilizes an assumed banded structure with given half-bandwidths, `mldq` and `mudq` (specified through `LowerBwidthDQ` and `UpperBwidthDQ`, respectively). However, the banded Jacobian block kept by the scheme has half-bandwidths `ml` and `mu` (specified through `LowerBwidth` and `UpperBwidth`), which may be smaller.

PrecSetupFn - Preconditioner setup function [function]
`PrecSetupFn` specifies an optional function which, together with `PrecSolve`, defines a right preconditioner matrix which is an approximation to the Newton matrix. `PrecSetupFn` must be of type `KINPrecSetupFn`.

PrecSolveFn - Preconditioner solve function [function]
`PrecSolveFn` specifies an optional function which must solve a linear system $Pz = r$, for given r . If `PrecSolveFn` is not defined, the no preconditioning will be used. `PrecSolveFn` must be of type `KINPrecSolveFn`.

GlocalFn - Local right-hand side approximation function for `BBDPre` [function]
If `PrecModule` is `BBDPre`, `GlocalFn` specifies a required function that evaluates a local approximation to the system function. `GlocalFn` must be of type `KINGlocalFn`.

GcommFn - Inter-process communication function for `BBDPre` [function]
If `PrecModule` is `BBDPre`, `GcommFn` specifies an optional function to perform any inter-process communication required for the evaluation of `GlocalFn`. `GcommFn` must be of type `KINGcommFn`.

LowerBwidth - Jacobian/preconditioner lower bandwidth [scalar | 0]
This property is overloaded. If the Band linear solver is used (see `LinSolver`), it specifies the lower half-bandwidth of the band Jacobian approximation. If one of the three iterative linear solvers, GMRES, BiCGStab, or TFQMR is used (see `LinSolver`) and if the `BBDPre` preconditioner module in KINSOL is used (see `PrecModule`), it specifies the lower half-bandwidth of the retained banded approximation of the local Jacobian block.

LowerBwidth defaults to 0 (no sub-diagonals).

UpperBwidth - Jacobian/preconditioner upper bandwidth [scalar | 0]
 This property is overloaded. If the Band linear solver is used (see LinSolver), it specifies the upper half-bandwidth of the band Jacobian approximation. If one of the three iterative linear solvers, GMRES, BiCGStab, or TFQMR is used (see LinSolver) and if the BBDDPre preconditioner module in KINSOL is used (see PrecModule), it specifies the upper half-bandwidth of the retained banded approximation of the local Jacobian block.
 UpperBwidth defaults to 0 (no super-diagonals).

LowerBwidthDQ - BBDDPre preconditioner DQ lower bandwidth [scalar | 0]
 Specifies the lower half-bandwidth used in the difference-quotient Jacobian approximation for the BBDDPre preconditioner (see PrecModule).

UpperBwidthDQ - BBDDPre preconditioner DQ upper bandwidth [scalar | 0]
 Specifies the upper half-bandwidth used in the difference-quotient Jacobian approximation for the BBDDPre preconditioner (see PrecModule).

Verbose - verbose output [true | false]
 Specifies whether or not KINSOL should output additional information

ErrorMessages - Post error/warning messages [false | true]
 Note that any errors in KINInit will result in a Matlab error, thus stopping execution. Only subsequent calls to KINSOL functions will respect the value specified for 'ErrorMessages'.

See also
 KINDenseJacFn, KINJacTimesVecFn
 KINPrecSetupFn, KINPrecSolveFn
 KINGlocalFn, KINGcommFn

KINInit

PURPOSE

KINInit allocates and initializes memory for KINSOL.

SYNOPSIS

```
function status = KINInit(fct, n, options)
```

DESCRIPTION

KINInit allocates and initializes memory for KINSOL.

Usage: KINInit (SYSFUN, N [, OPTIONS]);

SYSFUN is a function defining the nonlinear problem $f(y) = 0$.
 This function must return a column vector FY containing the current value of the residual

N is the (local) problem dimension.

OPTIONS is an (optional) set of integration options, created with the KINSetOptions function.

See also: KINSetOptions, KINSysFn

KINSol

PURPOSE

KINSol solves the nonlinear problem.

SYNOPSIS

```
function [status, y] = KINSol(y0, strategy, yscale, fscale)
```

DESCRIPTION

KINSol solves the nonlinear problem.

Usage: [STATUS, Y] = KINSol(Y0, STRATEGY, YSCALE, FSCALE)

KINSol manages the computational process of computing an approximate solution of the nonlinear system. If the initial guess (initial value assigned to vector Y0) doesn't violate any user-defined constraints, then KINSol attempts to solve the system $f(y)=0$. If an iterative linear solver was specified (see KINSetOptions), KINSol uses a nonlinear Krylov subspace projection method. The Newton-Krylov iterations are stopped if either of the following conditions is satisfied:

$$\|f(y)\|_{L\text{-infinity}} \leq 0.01 * \text{fnormtol}$$
$$\|y[i+1] - y[i]\|_{L\text{-infinity}} \leq \text{scsteptol}$$

However, if the current iterate satisfies the second stopping criterion, it doesn't necessarily mean an approximate solution has been found since the algorithm may have stalled, or the user-specified step tolerance may be too large.

STRATEGY specifies the global strategy applied to the Newton step if it is unsatisfactory. Valid choices are 'None' or 'LineSearch'.
YSCALE is a vector containing diagonal elements of scaling matrix for vector Y chosen so that the components of YSCALE*Y (as a matrix multiplication) all have about the same magnitude when Y is close to a root of $f(y)$.
FSCALE is a vector containing diagonal elements of scaling matrix for $f(y)$ chosen so that the components of FSCALE*f(Y) (as a matrix multiplication) all have roughly the same magnitude when u is not too near a root of $f(y)$.

On return, status is one of the following:

- 0: KINSol succeeded
- 1: The initial y0 already satisfies the stopping criterion given above
- 2: Stopping tolerance on scaled step length satisfied
- 1: An error occurred (see printed error message)

See also KINSetOptions, KINGetstats

KINGetStats

PURPOSE

KINGGetStats returns statistics for the main KINSOL solver and the linear

SYNOPSIS

```
function [si, status] = KINGGetStats()
```

DESCRIPTION

KINGGetStats returns statistics for the main KINSOL solver and the linear solver used.

Usage: STATS = KINGGetStats

Fields in the structure STATS

- o nfe - total number evaluations of the nonlinear system function SYSFUN
- o nni - total number of nonlinear iterations
- o nbcbf - total number of beta-condition failures
- o nbops - total number of backtrack operations (step length adjustments) performed by the line search algorithm
- o fnorm - scaled norm of the nonlinear system function $f(y)$ evaluated at the current iterate: $||f_{scale} * f(y)||_{L2}$
- o step - scaled norm (or length) of the step used during the previous iteration: $||u_{scale} * p||_{L2}$
- o LSInfo - structure with linear solver statistics

The structure LSInfo has different fields, depending on the linear solver used.

Fields in LSInfo for the 'Dense' linear solver

- o name - 'Dense'
- o njeD - number of Jacobian evaluations
- o nfeD - number of right-hand side function evaluations for difference-quotient Jacobian approximation

Fields in LSInfo for the 'GMRES' or 'BiCGStab' linear solver

- o name - 'GMRES' or 'BiCGStab'
- o nli - number of linear solver iterations
- o npe - number of preconditioner setups
- o nps - number of preconditioner solve function calls
- o ncfl - number of linear system convergence test failures

KINFree

PURPOSE

KINFree deallocates memory for the KINSOL solver.

SYNOPSIS

```
function KINFree()
```

DESCRIPTION

KINFree deallocates memory for the KINSOL solver.

Usage: KINFree

5.2 Function types

KINSysFn

PURPOSE

KINSysFn - type for user provided system function

SYNOPSIS

This is a script file.

DESCRIPTION

KINSysFn - type for user provided system function

The function SYSFUN must be defined as

FUNCTION [FY, FLAG] = SYSFUN(Y)

and must return a vector FY corresponding to $f(y)$.

If a user data structure DATA was specified in KINMalloc, then SYSFUN must be defined as

FUNCTION [FY, FLAG, NEW_DATA] = SYSFUN(Y,DATA)

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector FY, the SYSFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function SYSFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also KINMalloc

NOTE: SYSFUN is specified through the KINMalloc function.

KINDenseJacFn

PURPOSE

KINDenseJacFn - type for user provided dense Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

KINDenseJacFn - type for user provided dense Jacobian function.

The function DJACFUN must be defined as

FUNCTION [J, FLAG] = DJACFUN(Y,FY)

and must return a matrix J corresponding to the Jacobian of $f(y)$.

The input argument FY contains the current value of $f(y)$.
If a user data structure DATA was specified in KINMalloc, then DJACFUN must be defined as

```
FUNCTION [J, FLAG, NEW_DATA] = DJACFUN(Y,FY,DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J and the flag FLAG, the DJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function DJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also KINSetOptions

NOTE: DJACFUN is specified through the property JacobianFn to KINSetOptions and is used only if the property LinearSolver was set to 'Dense'.

KINBandJacFn

PURPOSE

KINBandJacFn - type for user provided banded Jacobian function.

SYNOPSIS

This is a script file.

DESCRIPTION

KINBandJacFn - type for user provided banded Jacobian function.

The function BJACFUN must be defined as

```
FUNCTION [J, FLAG] = BJACFUN(Y, FY)
```

and must return a matrix J corresponding to the banded Jacobian of $f(y)$.

The input argument FY contains the current value of $f(y)$.

If a user data structure DATA was specified in KINMalloc, then BJACFUN must be defined as

```
FUNCTION [J, FLAG, NEW_DATA] = BJACFUN(Y, FY, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the matrix J and the flag FLAG, the BJACFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function BJACFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also KINSetOptions

NOTE: BJACFUN is specified through the property JacobianFn to KINSetOptions and is used only if the property LinearSolver was set to 'Band'.

KINJacTimesVecFn

PURPOSE

KINJacTimesVecFn - type for user provided Jacobian times vector function.

SYNOPSIS

This is a script file.

DESCRIPTION

KINJacTimesVecFn - type for user provided Jacobian times vector function.

The function JTVFUN must be defined as

```
FUNCTION [JV, NEW_Y, FLAG] = JTVFUN(Y, V, NEW_Y)
```

and must return a vector JV corresponding to the product of the Jacobian of $f(y)$ with the vector v . On input, NEW_Y indicates if the iterate has been updated in the interim. JV must be update or reevaluated, if appropriate, unless NEW_Y=false. This flag must be reset by the user.

If a user data structure DATA was specified in KINMalloc, then JTVFUN must be defined as

```
FUNCTION [JV, NEW_Y, FLAG, NEW_DATA] = JTVFUN(Y, V, NEW_Y, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector JV, and flags NEW_Y and FLAG, the JTVFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

If successful, FLAG should be set to 0. If an error occurs, FLAG should be set to a nonzero value.

See also KINSetOptions

NOTE: JTVFUN is specified through the property JacobianFn to KINSetOptions and is used only if the property LinearSolver was set to 'GMRES' or 'BiCGStab'.

KINPrecSetupFn

PURPOSE

KINPrecSetupFn - type for user provided preconditioner setup function.

SYNOPSIS

This is a script file.

DESCRIPTION

KINPrecSetupFn - type for user provided preconditioner setup function.

The user-supplied preconditioner setup subroutine should compute the right-preconditioner matrix P used to form the scaled preconditioned linear system:

$$(Df * J(y) * (P^{-1}) * (Dy^{-1})) * (Dy * P * x) = Df * (-F(y))$$

where Dy and Df denote the diagonal scaling matrices whose diagonal elements are stored in the vectors `YSCALE` and `FSCALE`, respectively.

The preconditioner setup routine (referenced by iterative linear solver modules via `pset` (type `KINSpilsPrecSetupFn`)) will not be called prior to every call made to the `psolve` function, but will instead be called only as often as necessary to achieve convergence of the Newton iteration.

NOTE: If the `PRECSOLVE` function requires no preparation, then a preconditioner setup function need not be given.

The function `PSETFUN` must be defined as

```
FUNCTION FLAG = PSETFUN(Y, YSCALE, FY, FSCALE)
```

The input argument `FY` contains the current value of $f(y)$, while `YSCALE` and `FSCALE` are the scaling vectors for solution and system function, respectively (as passed to `KINSol`)

If a user data structure `DATA` was specified in `KINMalloc`, then `PSETFUN` must be defined as

```
FUNCTION [FLAG, NEW_DATA] = PSETFUN(Y, YSCALE, FY, FSCALE, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the flag `FLAG`, the `PSETFUN` function must also set `NEW_DATA`. Otherwise, it should set `NEW_DATA=[]` (do not set `NEW_DATA = DATA` as it would lead to unnecessary copying).

If successful, `PSETFUN` must return `FLAG=0`. For a recoverable error (in which case the setup will be retried) it must set `FLAG` to a positive integer value. If an unrecoverable error occurs, it must set `FLAG` to a negative value, in which case the solver will halt.

See also `KINPrecSolveFn`, `KINSetOptions`, `KINSol`

NOTE: `PSETFUN` is specified through the property `PrecSetupFn` to `KINSetOptions` and is used only if the property `LinearSolver` was set to `'GMRES'` or `'BiCGStab'`.

KINPrecSolveFn

PURPOSE

`KINPrecSolveFn` - type for user provided preconditioner solve function.

SYNOPSIS

This is a script file.

DESCRIPTION

KINPrecSolveFn - type for user provided preconditioner solve function.

The user-supplied preconditioner solve function PSOLFVN is to solve a linear system $Pz = r$ in which the matrix P is the preconditioner matrix (possibly set implicitly by PSETFUN)

The function PSOLFVN must be defined as

```
FUNCTION [Z, FLAG] = PSOLFVN(Y, YSCALE, FY, FSCALE, R)
```

and must return a vector Z containing the solution of $Pz=r$.

The input argument FY contains the current value of $f(y)$, while $YSCALE$ and $FSCALE$ are the scaling vectors for solution and system function, respectively (as passed to KINSol)

If a user data structure $DATA$ was specified in KINMalloc, then PSOLFVN must be defined as

```
FUNCTION [Z, FLAG, NEW_DATA] = PSOLFVN(Y, YSCALE, FY, FSCALE, R, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector Z and the flag $FLAG$, the PSOLFVN function must also set NEW_DATA . Otherwise, it should set $NEW_DATA=[]$ (do not set $NEW_DATA = DATA$ as it would lead to unnecessary copying).

If successful, PSOLFVN must return $FLAG=0$. For a recoverable error it must set $FLAG$ to a positive value (in which case the solver will attempt to correct). If an unrecoverable error occurs, it must set $FLAG$ to a negative value, in which case the solver will halt.

See also KINPrecSetupFn, KINSetOptions

NOTE: PSOLFVN is specified through the property PrecSolveFn to KINSetOptions and is used only if the property LinearSolver was set to 'GMRES' or 'BiCGStab'.

KINGcommFn

PURPOSE

KINGcommFn - type for user provided communication function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

KINGcommFn - type for user provided communication function (BBDPre).

The function GCOMFUN must be defined as

```
FUNCTION FLAG = GCOMFUN(Y)
```

and can be used to perform all interprocess communication necessary to evaluate the approximate right-hand side function for the BBDPre preconditioner module.

If a user data structure $DATA$ was specified in KINMalloc, then GCOMFUN must be defined as

```
FUNCTION [FLAG, NEW_DATA] = GCOMFUN(Y, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then the GCOMFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function GCOMFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also KINGlocalFn, KINSetOptions

NOTES:

GCOMFUN is specified through the GcommFn property in KINSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

Each call to GCOMFUN is preceded by a call to the system function SYSFUN with the same argument Y. Thus GCOMFUN can omit any communication done by SYSFUN if relevant to the evaluation of G by GLOCFUN. If all necessary communication was done by SYSFUN, GCOMFUN need not be provided.

KINGlocalFn

PURPOSE

KINGlocalFn - type for user provided RHS approximation function (BBDPre).

SYNOPSIS

This is a script file.

DESCRIPTION

KINGlocalFn - type for user provided RHS approximation function (BBDPre).

The function GLOCFUN must be defined as

```
FUNCTION [G, FLAG] = GLOCFUN(Y)
```

and must return a vector G corresponding to an approximation to f(y) which will be used in the BBDPRE preconditioner module. The case where G is mathematically identical to F is allowed.

If a user data structure DATA was specified in KINMalloc, then GLOCFUN must be defined as

```
FUNCTION [G, FLAG, NEW_DATA] = GLOCFUN(Y, DATA)
```

If the local modifications to the user data structure are needed in other user-provided functions then, besides setting the vector G, the GLOCFUN function must also set NEW_DATA. Otherwise, it should set NEW_DATA=[] (do not set NEW_DATA = DATA as it would lead to unnecessary copying).

The function GLOCFUN must set FLAG=0 if successful, FLAG<0 if an unrecoverable failure occurred, or FLAG>0 if a recoverable error occurred.

See also KINGcommFn, KINSetOptions

NOTE: GLOCFUN is specified through the GlocalFn property in KINSetOptions and is used only if the property PrecModule is set to 'BBDPre'.

6 Supporting modules

This section describes two additional modules in SUNDIALSTB, NVECTOR and PUTILS. The functions in NVECTOR perform various operations on vectors. For serial vectors, all of these operations default to the corresponding MATLAB functions. For parallel vectors, they can be used either on the local portion of the distributed vector or on the global vector (in which case they will trigger an MPI Allreduce operation). The functions in PUTILS are used to run parallel SUNDIALSTB applications. The user should only call the function `mpirun` to launch a parallel MATLAB application. See one of the parallel SUNDIALSTB examples for usage.

The functions in these two additional modules are listed in Table 10 and described in detail in the remainder of this section.

Table 10: The NVECTOR and PUTILS functions

NVECTOR	N_VMax	returns the largest element of x
	N_VMaxNorm	returns the maximum norm of x
	N_VMin	returns the smallest element of x
	N_VDotProd	returns the dot product of two vectors
	N_VWrmsNorm	returns the weighted root mean square norm of x
	N_VWL2Norm	returns the weighted Euclidean L2 norm of x
	N_VL1Norm	returns the L1 norm of x
PUTILS	mpirun	runs parallel examples
	mpiruns	runs the parallel example on a child MATLAB process
	mpistart	lamboot and <code>MPI_Init</code> master (if required)

6.1 NVECTOR functions

N_VDotProd

PURPOSE

N_VDotProd returns the dot product of two vectors

SYNOPSIS

```
function ret = N_VDotProd(x,y,comm)
```

DESCRIPTION

N_VDotProd returns the dot product of two vectors

Usage: RET = N_VDotProd (X, Y [, COMM])

If COMM is not present, N_VDotProd returns the dot product of the local portions of X and Y. Otherwise, it returns the global dot product.

SOURCE CODE

```
1 function ret = N_VDotProd(x,y,comm)
9
10 % Radu Serban <radu@llnl.gov>
11 % Copyright (c) 2005, The Regents of the University of California.
12 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
13
14
15 if nargin == 2
16
17     ret = dot(x,y);
18
19 else
20
21     ldot = dot(x,y);
22     gdot = 0.0;
23     MPI_Allreduce(ldot,gdot,'SUM',comm);
24     ret = gdot;
25
26 end
```

N_VL1Norm

PURPOSE

N_VL1Norm returns the L1 norm of x

SYNOPSIS

```
function ret = N_VL1Norm(x,comm)
```

DESCRIPTION

N_VL1Norm returns the L1 norm of x

Usage: RET = N_VL1Norm (X [, COMM])

If COMM is not present, N_VL1Norm returns the L1 norm of the local portion of X. Otherwise, it returns the global L1 norm..

SOURCE CODE

```
1 function ret = N_VL1Norm(x,comm)
9
10 % Radu Serban <radu@llnl.gov>
11 % Copyright (c) 2005, The Regents of the University of California.
12 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
13
14 if nargin == 1
15
16     ret = norm(x,1);
17
18 else
19
20     lnrn = norm(x,1);
21     gnrm = 0.0;
22     MPI_Allreduce(lnrm,gnrm,'MAX',comm);
23     ret = gnrm;
24
25 end
```

N_VMax

PURPOSE

N_VMax returns the largest element of x

SYNOPSIS

function ret = N_VMax(x,comm)

DESCRIPTION

N_VMax returns the largest element of x

Usage: RET = N_VMax (X [, COMM])

If COMM is not present, N_VMax returns the maximum value of the local portion of X. Otherwise, it returns the global maximum value.

SOURCE CODE

```
1 function ret = N_VMax(x,comm)
9
10 % Radu Serban <radu@llnl.gov>
11 % Copyright (c) 2005, The Regents of the University of California.
12 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
```

```

13
14 if nargin == 1
15
16     ret = max(x);
17
18 else
19
20     lmax = max(x);
21     gmax = 0.0;
22     MPI_Allreduce(lmax,gmax, 'MAX',comm);
23     ret = gmax;
24
25 end

```

N_VMaxNorm

PURPOSE

N_VMaxNorm returns the L-infinity norm of x

SYNOPSIS

```
function ret = N_VMaxNorm(x, comm)
```

DESCRIPTION

N_VMaxNorm returns the L-infinity norm of x

Usage: RET = N_VMaxNorm (X [, COMM])

If COMM is not present, N_VMaxNorm returns the L-infinity norm of the local portion of X. Otherwise, it returns the global L-infinity norm..

SOURCE CODE

```

1 function ret = N_VMaxNorm(x, comm)
9
10 % Radu Serban <radu@llnl.gov>
11 % Copyright (c) 2005, The Regents of the University of California.
12 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
13
14 if nargin == 1
15
16     ret = norm(x, 'inf');
17
18 else
19
20     lnrn = norm(x, 'inf');
21     gnrm = 0.0;
22     MPI_Allreduce(lnrm,gnrm, 'MAX',comm);
23     ret = gnrm;
24
25 end

```

N_VMin

PURPOSE

N_VMin returns the smallest element of x

SYNOPSIS

```
function ret = N_VMin(x,comm)
```

DESCRIPTION

N_VMin returns the smallest element of x

Usage: RET = N_VMin (X [, COMM])

If COMM is not present, N_VMin returns the minimum value of the local portion of X. Otherwise, it returns the global minimum value.

SOURCE CODE

```
1 function ret = N_VMin(x,comm)
2
3
4
5
6
7
8
9 % Radu Serban <radu@llnl.gov>
10 % Copyright (c) 2005, The Regents of the University of California.
11 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
12
13 if nargin == 1
14
15     ret = min(x);
16
17 else
18
19     lmin = min(x);
20     gmin = 0.0;
21     MPI_Allreduce(lmin,gmin,'MIN',comm);
22     ret = gmin;
23
24 end
```

N_VWL2Norm

PURPOSE

N_VWL2Norm returns the weighted Euclidean L2 norm of x

SYNOPSIS

```
function ret = N_VWL2Norm(x,w,comm)
```

DESCRIPTION

N_VWL2Norm returns the weighted Euclidean L2 norm of x
 with weight vector w:
 $\text{sqrt} \left[\left(\sum_{i=0}^{N-1} (x[i] * w[i])^2 \right) \right]$

Usage: RET = N_VWL2Norm (X, W [, COMM])

If COMM is not present, N_VWL2Norm returns the weighted L2 norm of the local portion of X. Otherwise, it returns the global weighted L2 norm..

SOURCE CODE

```

1 function ret = N_VWL2Norm(x,w,comm)
11
12 % Radu Serban <radu@llnl.gov>
13 % Copyright (c) 2005, The Regents of the University of California.
14 % $Revision: 1.1 $Date: 2006/01/06 19:00:10 $
15
16 if nargin == 2
17     ret = dot(x.^2,w.^2);
18     ret = sqrt(ret);
19
20
21 else
22
23     lnrn = dot(x.^2,w.^2);
24     gnrm = 0.0;
25     MPI_Allreduce(lnrm,gnrm,'SUM',comm);
26
27     ret = sqrt(gnrm);
28
29 end

```

N_VWrmsNorm

PURPOSE

N_VWrmsNorm returns the weighted root mean square norm of x

SYNOPSIS

function ret = N_VWrmsNorm(x,w,comm)

DESCRIPTION

N_VWrmsNorm returns the weighted root mean square norm of x
 with weight vector w:
 $\text{sqrt} \left[\left(\sum_{i=0}^{N-1} (x[i] * w[i])^2 \right) / N \right]$

Usage: RET = N_VWrmsNorm (X, W [, COMM])

If COMM is not present, N_VWrmsNorm returns the WRMS norm of the local portion of X. Otherwise, it returns the global WRMS norm..

SOURCE CODE

```

1  function ret = N_VWrmsNorm(x,w,comm)
11
12 % Radu Serban <radu@llnl.gov>
13 % Copyright (c) 2005, The Regents of the University of California.
14 % $Revision: 1.1 $Date: 2006/01/06 19:00:11 $
15
16 if nargin == 2
17
18     ret = dot(x.^2,w.^2);
19     ret = sqrt(ret/length(x));
20
21 else
22
23     lnrm = dot(x.^2,w.^2);
24     gnrm = 0.0;
25     MPI_Allreduce(lnrm,gnrm,'SUM',comm);
26
27     ln = length(x);
28     gn = 0;
29     MPI_Allreduce(ln,gn,'SUM',comm);
30
31     ret = sqrt(gnrm/gn);
32
33 end

```

6.2 Parallel utilities

mpirun

PURPOSE

MPIRUN runs parallel examples.

SYNOPSIS

```
function [] = mpirun(fct,npe,dbg)
```

DESCRIPTION

MPIRUN runs parallel examples.

Usage: MPIRUN (FCT , NPE [, DBG])

FCT - function to be executed on all MATLAB processes.

NPE - number of processes to be used (including the master).

DBG - flag for debugging [true | false]

If true, spawn MATLAB child processes with a visible xterm.

mpiruns

PURPOSE

MPIRUNS runs the parallel example on a child MATLAB process.

SYNOPSIS

```
function [] = mpiruns(fct)
```

DESCRIPTION

MPIRUNS runs the parallel example on a child MATLAB process.

Usage: MPIRUNS (FCT)

This function should not be called directly. It is called by mpirun on the spawned child processes.

mpistart

PURPOSE

MPISTART invokes lamboot (if required) and MPI_Init (if required).

SYNOPSIS

```
function mpistart(nslaves, rpi, hosts)
```

DESCRIPTION

MPISTART invokes lamboot (if required) and MPI_Init (if required).

Usage: MPISTART [(NSLAVES [, RPI [, HOSTS]])]

MPISTART boots LAM and initializes MPI to match a given number of slave hosts (and rpi) from a given list of hosts. All three args optional.

If they are not defined, HOSTS are taken from a builtin HOSTS list (edit HOSTS at the beginning of this file to match your cluster) or from the bhost file if defined through LAMBHOST (in this order).

If not defined, RPI is taken from the builtin variable RPI (edit it to suit your needs) or from the LAM_MPI_SSI_rpi environment variable (in this order).

A Implementation of CVMonitor.m

CVMonitor

PURPOSE

CVMonitor is the default CVMODES monitoring function.

SYNOPSIS

```
function [new_data] = CVMonitor(call, T, Y, YQ, YS, data)
```

DESCRIPTION

CVMonitor is the default CVMODES monitoring function.

To use it, set the Monitor property in CVMonitorOptions to 'CVMonitor' or to @CVMonitor and 'MonitorData' to mondata (defined as a structure).

With default settings, this function plots the evolution of the step size, method order, and various counters.

Various properties can be changed from their default values by passing to CVMonitorOptions, through the property 'MonitorData', a structure MONDATA with any of the following fields. If a field is not defined, the corresponding default value is used.

Fields in MONDATA structure:

- o stats [true | false]
If true, report the evolution of the step size and method order.
- o cntr [true | false]
If true, report the evolution of the following counters:
nst, nfe, nni, netf, ncnf (see CVMonitorGetStats)
- o mode ['graphical' | 'text' | 'both']
In graphical mode, plot the evolutions of the above quantities.
In text mode, print a table.
- o sol [true | false]
If true, plot solution components.
- o sensi [true | false]
If true and if FSA is enabled, plot sensitivity components.
- o select [array of integers]
To plot only particular solution components, specify their indices in the field select. If not defined, but sol=true, all components are plotted.
- o updt [integer | 50]
Update frequency. Data is posted in blocks of dimension n.
- o skip [integer | 0]
Number of integrations steps to skip in collecting data to post.
- o post [true | false]
If false, disable all posting. This option is necessary to disable monitoring on some processors when running in parallel.

See also CVMonitorOptions, CVMonitorFn

NOTES:

1. The argument mondata is REQUIRED. Even if only the default options are desired, set mondata=struct; and pass it to CVMonitorOptions.
2. The yQ argument is currently ignored.

SOURCE CODE

```

1 function [new_data] = CVMonitor(call, T, Y, YQ, YS, data)
45
46 % Radu Serban <radu@llnl.gov>
47 % Copyright (c) 2007, The Regents of the University of California.
48 % $Revision: 1.6 $Date: 2007/08/21 17:42:38 $
49
50 if (nargin ~= 6)
51     error('Monitor_data_not_defined. ');
52 end
53
54 new_data = [];
55
56 if call == 0
57
58 % Initialize unspecified fields to default values.
59     data = initialize_data(data);
60
61 % Open figure windows
62     if data.post
63
64         if data.grph
65             if data.stats | data.cntn
66                 data.hfg = figure;
67             end
68 %         Number of subplots in figure hfg
69             if data.stats
70                 data.npg = data.npg + 2;
71             end
72             if data.cntn
73                 data.npg = data.npg + 1;
74             end
75         end
76
77         if data.text
78             if data.cntn | data.stats
79                 data.hft = figure;
80             end
81         end
82
83         if data.sol | data.sensi
84             data.hfs = figure;
85         end
86
87     end
88
89 % Initialize other private data
90     data.i = 0;
91     data.n = 1;
92     data.t = zeros(1, data.updt);
93     if data.stats
94         data.h = zeros(1, data.updt);
95         data.q = zeros(1, data.updt);
96     end

```

```

97     if data.cntn
98         data.nst = zeros(1,data.updt);
99         data.nfe = zeros(1,data.updt);
100        data.nni = zeros(1,data.updt);
101        data.netf = zeros(1,data.updt);
102        data.ncfn = zeros(1,data.updt);
103    end
104
105    data.first = true;           % the next one will be the first call = 1
106    data.initialized = false; % the graphical windows were not initialized
107
108    new_data = data;
109
110    return;
111
112 else
113
114 % If this is the first call ~= 0,
115 % use Y and YS for additional initializations
116
117     if data.first
118
119         if isempty(YS)
120             data.sensi = false;
121         end
122
123         if data.sol | data.sensi
124
125             if isempty(data.select)
126
127                 data.N = length(Y);
128                 data.select = [1:data.N];
129
130             else
131
132                 data.N = length(data.select);
133
134             end
135
136             if data.sol
137                 data.y = zeros(data.N,data.updt);
138                 data.nps = data.nps + 1;
139             end
140
141             if data.sensi
142                 data.Ns = size(YS,2);
143                 data.ys = zeros(data.N, data.Ns, data.updt);
144                 data.nps = data.nps + data.Ns;
145             end
146
147         end
148
149         data.first = false;
150

```

```

151     end
152
153 % Extract variables from data
154
155     hfg = data.hfg;
156     hft = data.hft;
157     hfs = data.hfs;
158     npg = data.npg;
159     nps = data.nps;
160     i    = data.i;
161     n    = data.n;
162     t    = data.t;
163     N    = data.N;
164     Ns   = data.Ns;
165     y    = data.y;
166     ys   = data.ys;
167     h    = data.h;
168     q    = data.q;
169     nst  = data.nst;
170     nfe  = data.nfe;
171     nni  = data.nni;
172     netf = data.netf;
173     ncfm = data.ncfm;
174
175 end
176
177
178 % Load current statistics?
179
180 if call == 1
181
182     if i ~= 0
183         i = i - 1;
184         data.i = i;
185         new_data = data;
186         return;
187     end
188
189     si = CNodeGetStats;
190
191     t(n) = si.tcur;
192
193     if data.stats
194         h(n) = si.hlast;
195         q(n) = si.qlast;
196     end
197
198     if data.cntr
199         nst(n) = si.nst;
200         nfe(n) = si.nfe;
201         nni(n) = si.nni;
202         netf(n) = si.netf;
203         ncfm(n) = si.ncfm;
204     end

```

```

205
206 if data.sol
207     for j = 1:N
208         y(j,n) = Y(data.select(j));
209     end
210 end
211
212 if data.sensi
213     for k = 1:Ns
214         for j = 1:N
215             ys(j,k,n) = YS(data.select(j),k);
216         end
217     end
218 end
219
220 end
221
222 % Is it time to post?
223
224 if data.post & (n == data.updt | call==2)
225
226     if call == 2
227         n = n-1;
228     end
229
230     if ~data.initialized
231
232         if (data.stats | data.cntn) & data.grph
233             graphical_init(n, hfg, npg, data.stats, data.cntn, ...
234                 t, h, q, nst, nfe, nni, netf, ncf);
235         end
236
237         if (data.stats | data.cntn) & data.text
238             text_init(n, hft, data.stats, data.cntn, ...
239                 t, h, q, nst, nfe, nni, netf, ncf);
240         end
241
242         if data.sol | data.sensi
243             sol_init(n, hfs, nps, data.sol, data.sensi, ...
244                 N, Ns, t, y, ys);
245         end
246
247         data.initialized = true;
248
249     else
250
251         if (data.stats | data.cntn) & data.grph
252             graphical_update(n, hfg, npg, data.stats, data.cntn, ...
253                 t, h, q, nst, nfe, nni, netf, ncf);
254         end
255
256         if (data.stats | data.cntn) & data.text
257             text_update(n, hft, data.stats, data.cntn, ...
258                 t, h, q, nst, nfe, nni, netf, ncf);

```

```

259     end
260
261     if data.sol
262         sol_update(n, hfs, nps, data.sol, data.sensi, N, Ns, t, y, ys);
263     end
264
265 end
266
267 if call == 2
268
269     if (data.stats | data.cntr) & data.grph
270         graphical_final(hfg, npg, data.cntr, data.stats);
271     end
272
273     if data.sol | data.sensi
274         sol_final(hfs, nps, data.sol, data.sensi, N, Ns);
275     end
276
277     return;
278
279 end
280
281 n = 1;
282
283 else
284
285     n = n + 1;
286
287 end
288
289 % Save updated values in data
290
291 data.i      = data.skip;
292 data.n      = n;
293 data.npg    = npg;
294 data.t      = t;
295 data.y      = y;
296 data.ys     = ys;
297 data.h      = h;
298 data.q      = q;
299 data.nst    = nst;
300 data.nfe    = nfe;
301 data.nni    = nni;
302 data.netf   = netf;
303 data.ncfn   = ncfn;
304
305
306 new_data = data;
307
308 return;
309
310 %-----
311
312 function data = initialize_data(data)

```

```

313
314 if ~isfield(data, 'mode')
315     data.mode = 'graphical';
316 end
317 if ~isfield(data, 'updt')
318     data.updt = 50;
319 end
320 if ~isfield(data, 'skip')
321     data.skip = 0;
322 end
323 if ~isfield(data, 'stats')
324     data.stats = true;
325 end
326 if ~isfield(data, 'cntr')
327     data.cntr = true;
328 end
329 if ~isfield(data, 'sol')
330     data.sol = false;
331 end
332 if ~isfield(data, 'sensi')
333     data.sensi = false;
334 end
335 if ~isfield(data, 'select')
336     data.select = [];
337 end
338 if ~isfield(data, 'post')
339     data.post = true;
340 end
341
342 data.grph = true;
343 data.text = true;
344 if strcmp(data.mode, 'graphical')
345     data.text = false;
346 end
347 if strcmp(data.mode, 'text')
348     data.grph = false;
349 end
350
351 if ~data.sol & ~data.sensi
352     data.select = [];
353 end
354
355 % Other initializations
356 data.npg = 0;
357 data.nps = 0;
358 data.hfg = 0;
359 data.hft = 0;
360 data.hfs = 0;
361 data.h = 0;
362 data.q = 0;
363 data.nst = 0;
364 data.nfe = 0;
365 data.nni = 0;
366 data.netf = 0;

```



```

367 data.ncfn = 0;
368 data.N = 0;
369 data.Ns = 0;
370 data.y = 0;
371 data.ys = 0;
372
373 %-----
374
375 function [] = graphical_init(n, hfg, npg, stats, cntr, ...
376                             t, h, q, nst, nfe, nni, netf, ncfn)
377
378 fig_name = 'CVODES_run_statistics';
379
380 % If this is a parallel job, look for the MPI rank in the global
381 % workspace and append it to the figure name
382
383 global sundials_MPI_rank
384
385 if ~isempty(sundials_MPI_rank)
386     fig_name = sprintf('%s_(PE_%d)', fig_name, sundials_MPI_rank);
387 end
388
389 figure(hfg);
390 set(hfg, 'Name', fig_name);
391 set(hfg, 'color', [1 1 1]);
392 pl = 0;
393
394 % Time label and figure title
395
396 tlab = '\rightarrow nst \rightarrow';
397
398 % Step size and order
399 if stats
400     pl = pl+1;
401     subplot(npg, 1, pl)
402     semilogy(t(1:n), abs(h(1:n)), '-');
403     hold on;
404     box on;
405     grid on;
406     xlabel(tlab);
407     ylabel('|Step_size|');
408
409     pl = pl+1;
410     subplot(npg, 1, pl)
411     plot(t(1:n), q(1:n), '-');
412     hold on;
413     box on;
414     grid on;
415     xlabel(tlab);
416     ylabel('Order');
417 end
418
419 % Counters
420 if cntr

```

```

421     pl = pl+1;
422     subplot(npg,1,pl)
423     plot(t(1:n),nst(1:n),'k-');
424     hold on;
425     plot(t(1:n),nfe(1:n),'b-');
426     plot(t(1:n),nni(1:n),'r-');
427     plot(t(1:n),netf(1:n),'g-');
428     plot(t(1:n),ncfn(1:n),'c-');
429     box on;
430     grid on;
431     xlabel(tlab);
432     ylabel('Counters');
433 end
434
435 drawnow;
436
437 %-----
438
439 function [] = graphical_update(n, hfg, npg, stats, cntr, ...
440                               t, h, q, nst, nfe, nni, netf, ncfn)
441
442 figure(hfg);
443 pl = 0;
444
445 % Step size and order
446 if stats
447     pl = pl+1;
448     subplot(npg,1,pl)
449     hc = get(gca,'Children');
450     xd = [get(hc,'XData') t(1:n)];
451     yd = [get(hc,'YData') abs(h(1:n))];
452     set(hc,'XData',xd,'YData',yd);
453
454     pl = pl+1;
455     subplot(npg,1,pl)
456     hc = get(gca,'Children');
457     xd = [get(hc,'XData') t(1:n)];
458     yd = [get(hc,'YData') q(1:n)];
459     set(hc,'XData',xd,'YData',yd);
460 end
461
462 % Counters
463 if cntr
464     pl = pl+1;
465     subplot(npg,1,pl)
466     hc = get(gca,'Children');
467     % Attention: Children are loaded in reverse order!
468     xd = [get(hc(1),'XData') t(1:n)];
469     yd = [get(hc(1),'YData') ncfn(1:n)];
470     set(hc(1),'XData',xd,'YData',yd);
471     yd = [get(hc(2),'YData') netf(1:n)];
472     set(hc(2),'XData',xd,'YData',yd);
473     yd = [get(hc(3),'YData') nni(1:n)];
474     set(hc(3),'XData',xd,'YData',yd);

```

```

475     yd = [get(hc(4), 'YData') nfe(1:n)];
476     set(hc(4), 'XData', xd, 'YData', yd);
477     yd = [get(hc(5), 'YData') nst(1:n)];
478     set(hc(5), 'XData', xd, 'YData', yd);
479 end
480
481 drawnow;
482
483 %-----
484
485 function [] = graphical_final(hfg,npg,stats,cntr)
486
487 figure(hfg);
488 pl = 0;
489
490 if stats
491     pl = pl+1;
492     subplot(npg,1,pl)
493     hc = get(gca, 'Children');
494     xd = get(hc, 'XData');
495     set(gca, 'XLim', sort([xd(1) xd(end)]));
496
497     pl = pl+1;
498     subplot(npg,1,pl)
499     ylim = get(gca, 'YLim');
500     ylim(1) = ylim(1) - 1;
501     ylim(2) = ylim(2) + 1;
502     set(gca, 'YLim',ylim);
503     set(gca, 'XLim',sort([xd(1) xd(end)]));
504 end
505
506 if cntr
507     pl = pl+1;
508     subplot(npg,1,pl)
509     hc = get(gca, 'Children');
510     xd = get(hc(1), 'XData');
511     set(gca, 'XLim',sort([xd(1) xd(end)]));
512     legend('nst','nfe','nni','netf','ncfn',2);
513 end
514
515 %-----
516
517 function [] = text_init(n,hft,stats,cntr,t,h,q,nst,nfe,nni,netf,ncfn)
518
519 fig_name = 'CVODES_run_statistics';
520
521 % If this is a parallel job, look for the MPI rank in the global
522 % workspace and append it to the figure name
523
524 global sundials_MPI_rank
525
526 if ~isempty(sundials_MPI_rank)
527     fig_name = sprintf('%s_(PE_%d)',fig_name,sundials_MPI_rank);
528 end

```

```

529
530 figure(hft);
531 set(hft,'Name',fig_name);
532 set(hft,'color',[1 1 1]);
533 set(hft,'MenuBar','none');
534 set(hft,'Resize','off');
535
536 % Create text box
537
538 margins=[10 10 50 50]; % left, right, top, bottom
539 pos=get(hft,'position');
540 tbpos=[margins(1) margins(4) pos(3)-margins(1)-margins(2) ...
541        pos(4)-margins(3)-margins(4)];
542 tbpos(tbpos<1)=1;
543
544 htb=uicontrol(hft,'style','listbox','position',tbpos,'tag','textbox');
545 set(htb,'BackgroundColor',[1 1 1]);
546 set(htb,'SelectionHighlight','off');
547 set(htb,'FontName','courier');
548
549 % Create table head
550
551 tpos = [tbpos(1) tbpos(2)+tbpos(4)+10 tbpos(3) 20];
552 ht=uicontrol(hft,'style','text','position',tpos,'tag','text');
553 set(ht,'BackgroundColor',[1 1 1]);
554 set(ht,'HorizontalAlignment','left');
555 set(ht,'FontName','courier');
556 newline = '_____time_____step_____order____|_____nst_____nfe_____nni_____netf_____ncfn';
557 set(ht,'String',newline);
558
559 % Create OK button
560
561 bsize=[60,28];
562 badjustpos=[0,25];
563 bpos=[pos(3)/2-bsize(1)/2+badjustpos(1) -bsize(2)/2+badjustpos(2)...
564        bsize(1) bsize(2)];
565 bpos=round(bpos);
566 bpos(bpos<1)=1;
567 hb=uicontrol(hft,'style','pushbutton','position',bpos,...
568              'string','Close','tag','okaybutton');
569 set(hb,'callback','close');
570
571 % Save handles
572
573 handles=guihandles(hft);
574 guidata(hft,handles);
575
576 for i = 1:n
577     newline = '';
578     if stats
579         newline = sprintf('%10.3e____%10.3e_____1d____|',t(i),h(i),q(i));
580     end
581     if cntr
582         newline = sprintf('%s_%.5d_%.5d_%.5d_%.5d_%.5d',...

```

```

583         newline , nst(i) , nfe(i) , nni(i) , netf(i) , ncf(i));
584     end
585     string = get(handles.textbox , 'String');
586     string{end+1}=newline;
587     set(handles.textbox , 'String' , string);
588 end
589
590 drawnow
591
592 %-----
593
594 function [] = text_update(n,hft , stats , cntr , t , h , q , nst , nfe , nni , netf , ncf)
595
596 figure(hft);
597
598 handles=guidata(hft);
599
600 for i = 1:n
601     if stats
602         newline = sprintf( '%10.3e_%%10.3e_%%1d_%%' , t(i) , h(i) , q(i));
603     end
604     if cntr
605         newline = sprintf( '%s_%%5d_%%5d_%%5d_%%5d_%%5d' , ...
606                             newline , nst(i) , nfe(i) , nni(i) , netf(i) , ncf(i));
607     end
608     string = get(handles.textbox , 'String');
609     string{end+1}=newline;
610     set(handles.textbox , 'String' , string);
611 end
612
613 drawnow
614
615 %-----
616
617 function [] = sol_init(n, hfs , nps , sol , sensi , N, Ns, t , y , ys)
618
619 fig_name = 'CVODES_solution';
620
621 % If this is a parallel job, look for the MPI rank in the global
622 % workspace and append it to the figure name
623
624 global sundials_MPI_rank
625
626 if ~isempty(sundials_MPI_rank)
627     fig_name = sprintf( '%s_(PE_%%d)' , fig_name , sundials_MPI_rank);
628 end
629
630
631 figure(hfs);
632 set(hfs , 'Name' , fig_name);
633 set(hfs , 'color' , [1 1 1]);
634
635 % Time label
636

```

```

637 | tlab = '\rightarrow out \rightarrow';
638
639 | % Get number of colors in colormap
640 | map = colormap;
641 | ncols = size(map,1);
642
643 | % Initialize current subplot counter
644 | pl = 0;
645
646 | if sol
647
648 |     pl = pl+1;
649 |     subplot(nps,1,pl);
650 |     hold on;
651
652 |     for i = 1:N
653 |         hp = plot(t(1:n),y(i,1:n),'-');
654 |         ic = 1+(i-1)*floor(ncols/N);
655 |         set(hp,'Color',map(ic,:));
656 |     end
657 |     box on;
658 |     grid on;
659 |     xlabel(tlab);
660 |     ylabel('y');
661 |     title('Solution');
662
663 | end
664
665 | if sensi
666
667 |     for is = 1:Ns
668
669 |         pl = pl+1;
670 |         subplot(nps,1,pl);
671 |         hold on;
672
673 |         ys_crt = ys(:,is,1:n);
674 |         for i = 1:N
675 |             hp = plot(t(1:n),ys_crt(i,1:n),'-');
676 |             ic = 1+(i-1)*floor(ncols/N);
677 |             set(hp,'Color',map(ic,:));
678 |         end
679 |         box on;
680 |         grid on;
681 |         xlabel(tlab);
682 |         str = sprintf('s_{%d}',is); ylabel(str);
683 |         str = sprintf('Sensitivity_{%d}',is); title(str);
684
685 |     end
686
687 | end
688
689
690 | drawnow;

```

```

691 %
692 %
693
694 function [] = sol_update(n, hfs, nps, sol, sensi, N, Ns, t, y, ys)
695
696 figure(hfs);
697
698 pl = 0;
699
700 if sol
701
702     pl = pl+1;
703     subplot(nps,1,pl);
704
705     hc = get(gca, 'Children');
706     xd = [get(hc(1), 'XData') t(1:n)];
707     % Attention: Children are loaded in reverse order!
708     for i = 1:N
709         yd = [get(hc(i), 'YData') y(N-i+1,1:n)];
710         set(hc(i), 'XData', xd, 'YData', yd);
711     end
712
713 end
714
715 if sensi
716
717     for is = 1:Ns
718
719         pl = pl+1;
720         subplot(nps,1,pl);
721
722         ys_crt = ys(:,is,:);
723
724         hc = get(gca, 'Children');
725         xd = [get(hc(1), 'XData') t(1:n)];
726         % Attention: Children are loaded in reverse order!
727         for i = 1:N
728             yd = [get(hc(i), 'YData') ys_crt(N-i+1,1:n)];
729             set(hc(i), 'XData', xd, 'YData', yd);
730         end
731
732     end
733
734 end
735
736
737 drawnow;
738
739 %
740 %
741
742 function [] = sol_final(hfs, nps, sol, sensi, N, Ns)
743
744 figure(hfs);

```

```

745
746 pl = 0;
747
748 if sol
749
750     pl = pl +1;
751     subplot(nps,1,pl);
752
753     hc = get(gca,'Children');
754     xd = get(hc(1),'XData');
755     set(gca,'XLim',sort([xd(1) xd(end)]));
756
757     ylim = get(gca,'YLim');
758     addon = 0.1*abs(ylim(2)-ylim(1));
759     ylim(1) = ylim(1) + sign(ylim(1))*addon;
760     ylim(2) = ylim(2) + sign(ylim(2))*addon;
761     set(gca,'YLim',ylim);
762
763     for i = 1:N
764         cstring{i} = sprintf('y-{%d}',i);
765     end
766     legend(cstring);
767
768 end
769
770 if sensi
771
772     for is = 1:Ns
773
774         pl = pl+1;
775         subplot(nps,1,pl);
776
777         hc = get(gca,'Children');
778         xd = get(hc(1),'XData');
779         set(gca,'XLim',sort([xd(1) xd(end)]));
780
781         ylim = get(gca,'YLim');
782         addon = 0.1*abs(ylim(2)-ylim(1));
783         ylim(1) = ylim(1) + sign(ylim(1))*addon;
784         ylim(2) = ylim(2) + sign(ylim(2))*addon;
785         set(gca,'YLim',ylim);
786
787         for i = 1:N
788             cstring{i} = sprintf('s%d-{%d}',is,i);
789         end
790         legend(cstring);
791
792     end
793
794 end
795
796 drawnow

```

CVodeMonitorB

PURPOSE

CVodeMonitorB is the default CVODES monitoring function for backward problems.

SYNOPSIS

```
function [new_data] = CVodeMonitorB(call, idxB, T, Y, YQ, data)
```

DESCRIPTION

CVodeMonitorB is the default CVODES monitoring function for backward problems.

To use it, set the Monitor property in CVodeSetOptions to 'CVodeMonitorB' or to @CVodeMonitorB and 'MonitorData' to mondata (defined as a structure).

With default settings, this function plots the evolution of the step size, method order, and various counters.

Various properties can be changed from their default values by passing to CVodeSetOptions, through the property 'MonitorData', a structure MONDATA with any of the following fields. If a field is not defined, the corresponding default value is used.

Fields in MONDATA structure:

- o stats [true | false]
If true, report the evolution of the step size and method order.
- o cntr [true | false]
If true, report the evolution of the following counters:
nst, nfe, nni, netf, ncnf (see CVodeGetStats)
- o mode ['graphical' | 'text' | 'both']
In graphical mode, plot the evolutions of the above quantities.
In text mode, print a table.
- o sol [true | false]
If true, plot solution components.
- o select [array of integers]
To plot only particular solution components, specify their indeces in the field select. If not defined, but sol=true, all components are plotted.
- o updt [integer | 50]
Update frequency. Data is posted in blocks of dimension n.
- o skip [integer | 0]
Number of integrations steps to skip in collecting data to post.
- o post [true | false]
If false, disable all posting. This option is necessary to disable monitoring on some processors when running in parallel.

See also CVodeSetOptions, CVMonitorFnB

NOTES:

1. The argument mondata is REQUIRED. Even if only the default options are desired, set mondata=struct; and pass it to CVodeSetOptions.
2. The yQ argument is currently ignored.

B Implementation of IDAMonitor.m

IDAMonitor

PURPOSE

IDAMonitor is the default IDAS monitoring function.

SYNOPSIS

```
function [new_data] = IDAMonitor(call, T, Y, YQ, YS, data)
```

DESCRIPTION

IDAMonitor is the default IDAS monitoring function.

To use it, set the Monitor property in IDASetOptions to 'IDAMonitor' or to @IDAMonitor and 'MonitorData' to mondata (defined as a structure).

With default settings, this function plots the evolution of the step size, method order, and various counters.

Various properties can be changed from their default values by passing to IDASetOptions, through the property 'MonitorData', a structure MONDATA with any of the following fields. If a field is not defined, the corresponding default value is used.

Fields in MONDATA structure:

- o stats [true | false]
If true, report the evolution of the step size and method order.
- o cntr [true | false]
If true, report the evolution of the following counters:
nst, nfe, nni, netf, ncfn (see IDAGetStats)
- o mode ['graphical' | 'text' | 'both']
In graphical mode, plot the evolutions of the above quantities.
In text mode, print a table.
- o sol [true | false]
If true, plot solution components.
- o sensi [true | false]
If true and if FSA is enabled, plot sensitivity components.
- o select [array of integers]
To plot only particular solution components, specify their indices in the field select. If not defined, but sol=true, all components are plotted.
- o updt [integer | 50]
Update frequency. Data is posted in blocks of dimension n.
- o skip [integer | 0]
Number of integrations steps to skip in collecting data to post.
- o post [true | false]
If false, disable all posting. This option is necessary to disable monitoring on some processors when running in parallel.

See also IDASetOptions, IDAMonitorFn

NOTES:

1. The argument mondata is REQUIRED. Even if only the default options are desired, set mondata=struct; and pass it to IDASetOptions.
2. The yQ argument is currently ignored.

SOURCE CODE

```

1 function [new_data] = IDAMonitor(call, T, Y, YQ, YS, data)
45
46 % Radu Serban <radu@llnl.gov>
47 % Copyright (c) 2007, The Regents of the University of California.
48 % $Revision: 1.4 $Date: 2009/04/22 04:25:06 $
49
50 if (nargin ~= 6)
51     error('Monitor_data_not_defined. ');
52 end
53
54 new_data = [];
55
56 if call == 0
57
58 % Initialize unspecified fields to default values.
59     data = initialize_data(data);
60
61 % Open figure windows
62     if data.post
63
64         if data.grph
65             if data.stats | data.cntn
66                 data.hfg = figure;
67             end
68 %         Number of subplots in figure hfg
69             if data.stats
70                 data.npg = data.npg + 2;
71             end
72             if data.cntn
73                 data.npg = data.npg + 1;
74             end
75         end
76
77         if data.text
78             if data.cntn | data.stats
79                 data.hft = figure;
80             end
81         end
82
83         if data.sol | data.sensi
84             data.hfs = figure;
85         end
86
87     end
88
89 % Initialize other private data
90     data.i = 0;
91     data.n = 1;
92     data.t = zeros(1, data.updt);
93     if data.stats
94         data.h = zeros(1, data.updt);
95         data.q = zeros(1, data.updt);
96     end

```

```

97     if data.cntn
98         data.nst = zeros(1,data.updt);
99         data.nfe = zeros(1,data.updt);
100        data.nni = zeros(1,data.updt);
101        data.netf = zeros(1,data.updt);
102        data.ncfn = zeros(1,data.updt);
103    end
104
105    data.first = true;           % the next one will be the first call = 1
106    data.initialized = false; % the graphical windows were not initialized
107
108    new_data = data;
109
110    return;
111
112 else
113
114 % If this is the first call ~= 0,
115 % use Y and YS for additional initializations
116
117     if data.first
118
119         if isempty(YS)
120             data.sensi = false;
121         end
122
123         if data.sol | data.sensi
124
125             if isempty(data.select)
126
127                 data.N = length(Y);
128                 data.select = [1:data.N];
129
130             else
131
132                 data.N = length(data.select);
133
134             end
135
136             if data.sol
137                 data.y = zeros(data.N,data.updt);
138                 data.nps = data.nps + 1;
139             end
140
141             if data.sensi
142                 data.Ns = size(YS,2);
143                 data.ys = zeros(data.N, data.Ns, data.updt);
144                 data.nps = data.nps + data.Ns;
145             end
146
147         end
148
149         data.first = false;
150

```

```

151     end
152
153 % Extract variables from data
154
155     hfg = data.hfg;
156     hft = data.hft;
157     hfs = data.hfs;
158     npg = data.npg;
159     nps = data.nps;
160     i    = data.i;
161     n    = data.n;
162     t    = data.t;
163     N    = data.N;
164     Ns   = data.Ns;
165     y    = data.y;
166     ys   = data.ys;
167     h    = data.h;
168     q    = data.q;
169     nst  = data.nst;
170     nfe  = data.nfe;
171     nni  = data.nni;
172     netf = data.netf;
173     ncfm = data.ncfm;
174
175 end
176
177
178 % Load current statistics?
179
180 if call == 1
181
182     if i ~= 0
183         i = i - 1;
184         data.i = i;
185         new_data = data;
186         return;
187     end
188
189     si = IDAGetStats;
190
191     t(n) = si.tcur;
192
193     if data.stats
194         h(n) = si.hlast;
195         q(n) = si.qlast;
196     end
197
198     if data.cntr
199         nst(n) = si.nst;
200         nfe(n) = si.nfe;
201         nni(n) = si.nni;
202         netf(n) = si.netf;
203         ncfm(n) = si.ncfm;
204     end

```

```

205
206 if data.sol
207     for j = 1:N
208         y(j,n) = Y(data.select(j));
209     end
210 end
211
212 if data.sensi
213     for k = 1:Ns
214         for j = 1:N
215             ys(j,k,n) = YS(data.select(j),k);
216         end
217     end
218 end
219
220 end
221
222 % Is it time to post?
223
224 if data.post & (n == data.updt | call==2)
225
226     if call == 2
227         n = n-1;
228     end
229
230     if ~data.initialized
231
232         if (data.stats | data.cntn) & data.grph
233             graphical_init(n, hfg, npg, data.stats, data.cntn, ...
234                 t, h, q, nst, nfe, nni, netf, ncf);
235         end
236
237         if (data.stats | data.cntn) & data.text
238             text_init(n, hft, data.stats, data.cntn, ...
239                 t, h, q, nst, nfe, nni, netf, ncf);
240         end
241
242         if data.sol | data.sensi
243             sol_init(n, hfs, nps, data.sol, data.sensi, ...
244                 N, Ns, t, y, ys);
245         end
246
247         data.initialized = true;
248
249     else
250
251         if (data.stats | data.cntn) & data.grph
252             graphical_update(n, hfg, npg, data.stats, data.cntn, ...
253                 t, h, q, nst, nfe, nni, netf, ncf);
254         end
255
256         if (data.stats | data.cntn) & data.text
257             text_update(n, hft, data.stats, data.cntn, ...
258                 t, h, q, nst, nfe, nni, netf, ncf);

```

```

259     end
260
261     if data.sol
262         sol_update(n, hfs, nps, data.sol, data.sensi, N, Ns, t, y, ys);
263     end
264
265 end
266
267 if call == 2
268
269     if (data.stats | data.cntr) & data.grph
270         graphical_final(hfg, npg, data.cntr, data.stats);
271     end
272
273     if data.sol | data.sensi
274         sol_final(hfs, nps, data.sol, data.sensi, N, Ns);
275     end
276
277     return;
278
279 end
280
281 n = 1;
282
283 else
284
285     n = n + 1;
286
287 end
288
289 % Save updated values in data
290
291 data.i      = data.skip;
292 data.n      = n;
293 data.npg    = npg;
294 data.t      = t;
295 data.y      = y;
296 data.ys     = ys;
297 data.h      = h;
298 data.q      = q;
299 data.nst    = nst;
300 data.nfe    = nfe;
301 data.nni    = nni;
302 data.netf   = netf;
303 data.ncfn   = ncfn;
304
305
306 new_data = data;
307
308 return;
309
310 %-----
311
312 function data = initialize_data(data)

```

```

313
314 if ~isfield(data, 'mode')
315     data.mode = 'graphical';
316 end
317 if ~isfield(data, 'updt')
318     data.updt = 50;
319 end
320 if ~isfield(data, 'skip')
321     data.skip = 0;
322 end
323 if ~isfield(data, 'stats')
324     data.stats = true;
325 end
326 if ~isfield(data, 'cntr')
327     data.cntr = true;
328 end
329 if ~isfield(data, 'sol')
330     data.sol = false;
331 end
332 if ~isfield(data, 'sensi')
333     data.sensi = false;
334 end
335 if ~isfield(data, 'select')
336     data.select = [];
337 end
338 if ~isfield(data, 'post')
339     data.post = true;
340 end
341
342 data.grph = true;
343 data.text = true;
344 if strcmp(data.mode, 'graphical')
345     data.text = false;
346 end
347 if strcmp(data.mode, 'text')
348     data.grph = false;
349 end
350
351 if ~data.sol & ~data.sensi
352     data.select = [];
353 end
354
355 % Other initializations
356 data.npg = 0;
357 data.nps = 0;
358 data.hfg = 0;
359 data.hft = 0;
360 data.hfs = 0;
361 data.h = 0;
362 data.q = 0;
363 data.nst = 0;
364 data.nfe = 0;
365 data.nni = 0;
366 data.netf = 0;

```



```

367 data.ncfn = 0;
368 data.N = 0;
369 data.Ns = 0;
370 data.y = 0;
371 data.ys = 0;
372
373 %-----
374
375 function [] = graphical_init(n, hfg, npg, stats, cntr, ...
376                             t, h, q, nst, nfe, nni, netf, ncfn)
377
378 fig_name = 'IDAS_run_statistics';
379
380 % If this is a parallel job, look for the MPI rank in the global
381 % workspace and append it to the figure name
382
383 global sundials_MPI_rank
384
385 if ~isempty(sundials_MPI_rank)
386     fig_name = sprintf( '%s_(PE_%d)', fig_name, sundials_MPI_rank);
387 end
388
389 figure(hfg);
390 set(hfg, 'Name', fig_name);
391 set(hfg, 'color', [1 1 1]);
392 pl = 0;
393
394 % Time label and figure title
395
396 tlab = '\rightarrow t \rightarrow';
397
398 % Step size and order
399 if stats
400     pl = pl+1;
401     subplot(npg,1,pl)
402     semilogy(t(1:n),abs(h(1:n)),'-');
403     hold on;
404     box on;
405     grid on;
406     xlabel(tlab);
407     ylabel(' | Step_size | ');
408
409     pl = pl+1;
410     subplot(npg,1,pl)
411     plot(t(1:n),q(1:n),'-');
412     hold on;
413     box on;
414     grid on;
415     xlabel(tlab);
416     ylabel(' Order ');
417 end
418
419 % Counters
420 if cntr

```

```

421     pl = pl+1;
422     subplot(npg,1,pl)
423     plot(t(1:n),nst(1:n),'k-');
424     hold on;
425     plot(t(1:n),nfe(1:n),'b-');
426     plot(t(1:n),nni(1:n),'r-');
427     plot(t(1:n),netf(1:n),'g-');
428     plot(t(1:n),ncfn(1:n),'c-');
429     box on;
430     grid on;
431     xlabel(tlab);
432     ylabel('Counters');
433 end
434
435 drawnow;
436
437 %-----
438
439 function [] = graphical_update(n, hfg, npg, stats, cntr, ...
440                               t, h, q, nst, nfe, nni, netf, ncfn)
441
442 figure(hfg);
443 pl = 0;
444
445 % Step size and order
446 if stats
447     pl = pl+1;
448     subplot(npg,1,pl)
449     hc = get(gca,'Children');
450     xd = [get(hc,'XData') t(1:n)];
451     yd = [get(hc,'YData') abs(h(1:n))];
452     set(hc,'XData',xd,'YData',yd);
453
454     pl = pl+1;
455     subplot(npg,1,pl)
456     hc = get(gca,'Children');
457     xd = [get(hc,'XData') t(1:n)];
458     yd = [get(hc,'YData') q(1:n)];
459     set(hc,'XData',xd,'YData',yd);
460 end
461
462 % Counters
463 if cntr
464     pl = pl+1;
465     subplot(npg,1,pl)
466     hc = get(gca,'Children');
467     % Attention: Children are loaded in reverse order!
468     xd = [get(hc(1),'XData') t(1:n)];
469     yd = [get(hc(1),'YData') ncfn(1:n)];
470     set(hc(1),'XData',xd,'YData',yd);
471     yd = [get(hc(2),'YData') netf(1:n)];
472     set(hc(2),'XData',xd,'YData',yd);
473     yd = [get(hc(3),'YData') nni(1:n)];
474     set(hc(3),'XData',xd,'YData',yd);

```

```

475     yd = [get(hc(4), 'YData') nfe(1:n)];
476     set(hc(4), 'XData', xd, 'YData', yd);
477     yd = [get(hc(5), 'YData') nst(1:n)];
478     set(hc(5), 'XData', xd, 'YData', yd);
479 end
480
481 drawnow;
482
483 %-----
484
485 function [] = graphical_final(hfg, npg, stats, cntr)
486
487 figure(hfg);
488 pl = 0;
489
490 if stats
491     pl = pl+1;
492     subplot(npg,1,pl)
493     hc = get(gca, 'Children');
494     xd = get(hc, 'XData');
495     set(gca, 'XLim', sort([xd(1) xd(end)]));
496
497     pl = pl+1;
498     subplot(npg,1,pl)
499     ylim = get(gca, 'YLim');
500     ylim(1) = ylim(1) - 1;
501     ylim(2) = ylim(2) + 1;
502     set(gca, 'YLim', ylim);
503     set(gca, 'XLim', sort([xd(1) xd(end)]));
504 end
505
506 if cntr
507     pl = pl+1;
508     subplot(npg,1,pl)
509     hc = get(gca, 'Children');
510     xd = get(hc(1), 'XData');
511     set(gca, 'XLim', sort([xd(1) xd(end)]));
512     legend('nst', 'nfe', 'nni', 'netf', 'ncfn', 2);
513 end
514
515 %-----
516
517 function [] = text_init(n, hft, stats, cntr, t, h, q, nst, nfe, nni, netf, ncfn)
518
519 fig_name = 'IDAS_run_statistics';
520
521 % If this is a parallel job, look for the MPI rank in the global
522 % workspace and append it to the figure name
523
524 global sundials_MPI_rank
525
526 if ~isempty(sundials_MPI_rank)
527     fig_name = sprintf('%s_(PE_%d)', fig_name, sundials_MPI_rank);
528 end

```

```

529
530 figure(hft);
531 set(hft,'Name',fig_name);
532 set(hft,'color',[1 1 1]);
533 set(hft,'MenuBar','none');
534 set(hft,'Resize','off');
535
536 % Create text box
537
538 margins=[10 10 50 50]; % left, right, top, bottom
539 pos=get(hft,'position');
540 tbpos=[margins(1) margins(4) pos(3)-margins(1)-margins(2) ...
541        pos(4)-margins(3)-margins(4)];
542 tbpos(tbpos<1)=1;
543
544 htb=uicontrol(hft,'style','listbox','position',tbpos,'tag','textbox');
545 set(htb,'BackgroundColor',[1 1 1]);
546 set(htb,'SelectionHighlight','off');
547 set(htb,'FontName','courier');
548
549 % Create table head
550
551 tpos = [tbpos(1) tbpos(2)+tbpos(4)+10 tbpos(3) 20];
552 ht=uicontrol(hft,'style','text','position',tpos,'tag','text');
553 set(ht,'BackgroundColor',[1 1 1]);
554 set(ht,'HorizontalAlignment','left');
555 set(ht,'FontName','courier');
556 newline = 'time step order | inst fe nni netf ncfn';
557 set(ht,'String',newline);
558
559 % Create OK button
560
561 bsize=[60,28];
562 badjustpos=[0,25];
563 bpos=[pos(3)/2-bsize(1)/2+badjustpos(1) -bsize(2)/2+badjustpos(2)...
564        bsize(1) bsize(2)];
565 bpos=round(bpos);
566 bpos(bpos<1)=1;
567 hb=uicontrol(hft,'style','pushbutton','position',bpos,...
568              'string','Close','tag','okaybutton');
569 set(hb,'callback','close');
570
571 % Save handles
572
573 handles=guihandles(hft);
574 guidata(hft,handles);
575
576 for i = 1:n
577     newline = '';
578     if stats
579         newline = sprintf('%10.3e %10.3e %1d | ',t(i),h(i),q(i));
580     end
581     if cntr
582         newline = sprintf('%s %5d %5d %5d %5d %5d',...

```

```

583         newline , nst(i) , nfe(i) , nni(i) , netf(i) , ncf(i));
584     end
585     string = get(handles.textbox , 'String');
586     string{end+1}=newline;
587     set(handles.textbox , 'String' , string);
588 end
589
590 drawnow
591
592 %-----
593
594 function [] = text_update(n,hft , stats , cntr , t , h , q , nst , nfe , nni , netf , ncf(i))
595
596 figure(hft);
597
598 handles=guidata(hft);
599
600 for i = 1:n
601     if stats
602         newline = sprintf( '%10.3e_%%10.3e_%%1d_%%' , t(i) , h(i) , q(i));
603     end
604     if cntr
605         newline = sprintf( '%s_%%5d_%%5d_%%5d_%%5d_%%5d' , ...
606                             newline , nst(i) , nfe(i) , nni(i) , netf(i) , ncf(i));
607     end
608     string = get(handles.textbox , 'String');
609     string{end+1}=newline;
610     set(handles.textbox , 'String' , string);
611 end
612
613 drawnow
614
615 %-----
616
617 function [] = sol_init(n, hfs , nps , sol , sensi , N, Ns, t , y , ys)
618
619 fig_name = 'IDAS_solution';
620
621 % If this is a parallel job, look for the MPI rank in the global
622 % workspace and append it to the figure name
623
624 global sundials_MPI_rank
625
626 if ~isempty(sundials_MPI_rank)
627     fig_name = sprintf( '%s_(PE_%%d)' , fig_name , sundials_MPI_rank);
628 end
629
630
631 figure(hfs);
632 set(hfs , 'Name' , fig_name);
633 set(hfs , 'color' , [1 1 1]);
634
635 % Time label
636

```

```

637 | tlab = '\rightarrow out \rightarrow';
638 |
639 | % Get number of colors in colormap
640 | map = colormap;
641 | ncols = size(map,1);
642 |
643 | % Initialize current subplot counter
644 | pl = 0;
645 |
646 | if sol
647 |
648 |     pl = pl+1;
649 |     subplot(nps,1,pl);
650 |     hold on;
651 |
652 |     for i = 1:N
653 |         hp = plot(t(1:n),y(i,1:n),'-');
654 |         ic = 1+(i-1)*floor(ncols/N);
655 |         set(hp,'Color',map(ic,:));
656 |     end
657 |     box on;
658 |     grid on;
659 |     xlabel(tlab);
660 |     ylabel('y');
661 |     title('Solution');
662 |
663 | end
664 |
665 | if sensi
666 |
667 |     for is = 1:Ns
668 |
669 |         pl = pl+1;
670 |         subplot(nps,1,pl);
671 |         hold on;
672 |
673 |         ys_crt = ys(:,is,1:n);
674 |         for i = 1:N
675 |             hp = plot(t(1:n),ys_crt(i,1:n),'-');
676 |             ic = 1+(i-1)*floor(ncols/N);
677 |             set(hp,'Color',map(ic,:));
678 |         end
679 |         box on;
680 |         grid on;
681 |         xlabel(tlab);
682 |         str = sprintf('s_{%d}',is); ylabel(str);
683 |         str = sprintf('Sensitivity_{%d}',is); title(str);
684 |
685 |     end
686 |
687 | end
688 |
689 |
690 | drawnow;

```

```

691 %
692 %
693
694 function [] = sol_update(n, hfs, nps, sol, sensi, N, Ns, t, y, ys)
695
696 figure(hfs);
697
698 pl = 0;
699
700 if sol
701
702     pl = pl+1;
703     subplot(nps,1,pl);
704
705     hc = get(gca, 'Children');
706     xd = [get(hc(1), 'XData') t(1:n)];
707     % Attention: Children are loaded in reverse order!
708     for i = 1:N
709         yd = [get(hc(i), 'YData') y(N-i+1,1:n)];
710         set(hc(i), 'XData', xd, 'YData', yd);
711     end
712
713 end
714
715 if sensi
716
717     for is = 1:Ns
718
719         pl = pl+1;
720         subplot(nps,1,pl);
721
722         ys_crt = ys(:,is,:);
723
724         hc = get(gca, 'Children');
725         xd = [get(hc(1), 'XData') t(1:n)];
726         % Attention: Children are loaded in reverse order!
727         for i = 1:N
728             yd = [get(hc(i), 'YData') ys_crt(N-i+1,1:n)];
729             set(hc(i), 'XData', xd, 'YData', yd);
730         end
731
732     end
733
734 end
735
736
737 drawnow;
738
739 %
740 %
741
742 function [] = sol_final(hfs, nps, sol, sensi, N, Ns)
743
744 figure(hfs);

```

```

745
746 pl = 0;
747
748 if sol
749
750     pl = pl + 1;
751     subplot(nps,1,pl);
752
753     hc = get(gca,'Children');
754     xd = get(hc(1),'XData');
755     set(gca,'XLim',sort([xd(1) xd(end)]));
756
757     ylim = get(gca,'YLim');
758     addon = 0.1*abs(ylim(2)-ylim(1));
759     ylim(1) = ylim(1) + sign(ylim(1))*addon;
760     ylim(2) = ylim(2) + sign(ylim(2))*addon;
761     set(gca,'YLim',ylim);
762
763     for i = 1:N
764         cstring{i} = sprintf('y-{%d}',i);
765     end
766     legend(cstring);
767
768 end
769
770 if sensi
771
772     for is = 1:Ns
773
774         pl = pl+1;
775         subplot(nps,1,pl);
776
777         hc = get(gca,'Children');
778         xd = get(hc(1),'XData');
779         set(gca,'XLim',sort([xd(1) xd(end)]));
780
781         ylim = get(gca,'YLim');
782         addon = 0.1*abs(ylim(2)-ylim(1));
783         ylim(1) = ylim(1) + sign(ylim(1))*addon;
784         ylim(2) = ylim(2) + sign(ylim(2))*addon;
785         set(gca,'YLim',ylim);
786
787         for i = 1:N
788             cstring{i} = sprintf('s%d-{%d}',is,i);
789         end
790         legend(cstring);
791
792     end
793
794 end
795
796 drawnow

```

IDAMonitorB

PURPOSE

IDAMonitorB is the default IDAS monitoring function for backward problems.

SYNOPSIS

```
function [new_data] = IDAMonitorB(call, idxB, T, Y, YQ, data)
```

DESCRIPTION

IDAMonitorB is the default IDAS monitoring function for backward problems.

To use it, set the Monitor property in IDASetOptions to 'IDAMonitorB' or to @IDAMonitorB and 'MonitorData' to mondata (defined as a structure).

With default settings, this function plots the evolution of the step size, method order, and various counters.

Various properties can be changed from their default values by passing to IDASetOptions, through the property 'MonitorData', a structure MONDATA with any of the following fields. If a field is not defined, the corresponding default value is used.

Fields in MONDATA structure:

- o stats [true | false]
If true, report the evolution of the step size and method order.
- o cntr [true | false]
If true, report the evolution of the following counters:
nst, nfe, nni, netf, ncf (see IDAGetStats)
- o mode ['graphical' | 'text' | 'both']
In graphical mode, plot the evolutions of the above quantities.
In text mode, print a table.
- o sol [true | false]
If true, plot solution components.
- o select [array of integers]
To plot only particular solution components, specify their indices in the field select. If not defined, but sol=true, all components are plotted.
- o updt [integer | 50]
Update frequency. Data is posted in blocks of dimension n.
- o skip [integer | 0]
Number of integrations steps to skip in collecting data to post.
- o post [true | false]
If false, disable all posting. This option is necessary to disable monitoring on some processors when running in parallel.

See also IDASetOptions, IDAMonitorFnB

NOTES:

1. The argument mondata is REQUIRED. Even if only the default options are desired, set mondata=struct; and pass it to IDASetOptions.
2. The yQ argument is currently ignored.

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- [3] A. C. Hindmarsh and R. Serban. User Documentation for CVODES v2.6.0. Technical report, LLNL, 2009. UCRL-SM-208111.
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