User Documentation for IDAS v2.0.0 (SUNDIALS v3.0.0)

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Introduction

IDAS is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [20]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities, CVODES and IDAS.

IDAS is a general purpose solver for the initial value problem (IVP) for systems of differential-algebraic equations (DAEs). The name IDAS stands for Implicit Differential-Algebraic solver with Sensitivity capabilities. IDAS is an extension of the IDA solver within SUNDIALS, itself based on DASPK [5, 6]; however, like all SUNDIALS solvers, IDAS is written in ANSI-standard C rather than FORTRAN77. Its most notable features are that, (1) in the solution of the underlying nonlinear system at each time step, it offers a choice of Newton/direct methods and a choice of Inexact Newton/Krylov (iterative) methods; (2) it is written in a *data-independent* manner in that it acts on generic vectors without any assumptions on the underlying organization of the data; and (3) it provides a flexible, extensible framework for sensitivity analysis, using either *forward* or *adjoint* methods. Thus IDAS shares significant modules previously written within CASC at LLNL to support the ordinary differential equation (ODE) solvers CVODE [21, 12] and PVODE [8, 9], the DAE solver IDA [24] on which IDAS is based, the sensitivity-enabled ODE solver CVODES [22, 34], and also the nonlinear system solver KINSOL [13].

The Newton/Krylov methods in IDAS are: the GMRES (Generalized Minimal RESidual) [33], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [36], and TFQMR (Transpose-Free Quasi-Minimal Residual) linear iterative methods [17]. As Krylov methods, these require almost no matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner matrix, and for most problems preconditioning is essential for an efficient solution.

For very large DAE systems, the Krylov methods are preferable over direct linear solver methods, and are often the only feasible choice. Among the three Krylov methods in IDAS, we recommend GMRES as the best overall choice. However, users are encouraged to compare all three, especially if encountering convergence failures with GMRES. Bi-CGFStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size.

IDAS is written with a functionality that is a superset of that of IDA. Sensitivity analysis capabilities, both forward and adjoint, have been added to the main integrator. Enabling forward sensitivity computations in IDAS will result in the code integrating the so-called *sensitivity equations* simultaneously with the original IVP, yielding both the solution and its sensitivity with respect to parameters in the model. Adjoint sensitivity analysis, most useful when the gradients of relatively few functionals of the solution with respect to many parameters are sought, involves integration of the original IVP forward in time followed by the integration of the so-called *adjoint equations* backward in time. IDAS provides the infrastructure needed to integrate any final-condition ODE dependent on the solution of the original IVP (in particular the adjoint system).

There are several motivations for choosing the C language for IDAS. First, a general movement away from FORTRAN and toward C in scientific computing was apparent. Second, the pointer, structure,

and dynamic memory allocation features in C are extremely useful in software of this complexity, with the great variety of method options offered. Finally, we prefer C over C++ for IDAS because of the wider availability of C compilers, the potentially greater efficiency of C, and the greater ease of interfacing the solver to applications written in extended FORTRAN.

1.1 Changes from previous versions

Changes in v2.0.0

All interfaces to matrix structures and linear solvers have been reworked, and all example programs have been updated. The goal of the redesign of these interfaces was to provide more encapsulation and ease interfacing of custom linear solvers and interoperability with linear solver libraries. Specific changes include:

- Added generic SUNMATRIX module with three provided implementations: dense, banded and sparse. These replicate previous SUNDIALS Dls and Sls matrix structures in a single object-oriented API.
- Added example problems demonstrating use of generic SUNMATRIX modules.
- Added generic SUNLINEARSOLVER module with eleven provided implementations: dense, banded, LAPACK dense, LAPACK band, KLU, SuperLU_MT, SPGMR, SPBCGS, SPTFQMR, SPFGMR, PCG. These replicate previous SUNDIALS generic linear solvers in a single object-oriented API.
- Added example problems demonstrating use of generic SUNLINEARSOLVER modules.
- Expanded package-provided direct linear solver (Dls) interfaces and scaled, preconditioned, iterative linear solver (Spils) interfaces to utilize generic SUNMATRIX and SUNLINEARSOLVER objects.
- Removed package-specific, linear solver-specific, solver modules (e.g. CVDENSE, KINBAND, IDAKLU, ARKSPGMR) since their functionality is entirely replicated by the generic Dls/Spils interfaces and SUNLINEARSOLVER/SUNMATRIX modules. The exception is CVDIAG, a diagonal approximate Jacobian solver available to CVODE and CVODES.
- Converted all SUNDIALS example problems to utilize new generic SUNMATRIX and SUNLINEARSOLVER objects, along with updated Dls and Spils linear solver interfaces.
- Added Spils interface routines to ARKode, CVODE, CVODES, IDA and IDAS to allow specification of a user-provided "JTSetup" routine. This change supports users who wish to set up data structures for the user-provided Jacobian-times-vector ("JTimes") routine, and where the cost of one JTSetup setup per Newton iteration can be amortized between multiple JTimes calls.

Two additional NVECTOR implementations were added – one for CUDA and one for RAJA vectors. These vectors are supplied to provide very basic support for running on GPU architectures. Users are advised that these vectors both move all data to the GPU device upon construction, and speedup will only be realized if the user also conducts the right-hand-side function evaluation on the device. In addition, these vectors assume the problem fits on one GPU. Further information about RAJA, users are referred to the web site, https://software.llnl.gov/RAJA/. These additions are accompanied by additions to various interface functions and to user documentation.

All indices for data structures were updated to a new sunindextype that can be configured to be a 32- or 64-bit integer data index type. Sunindextype can be defined to be int64_t or int32_t or long long int and int depending on machine support for portable types. Fortran interfaces only support long int This new flexible capability for index types includes interfaces to PETSc, hypre, SuperLU_MT, and KLU with either 64-bit or 32-bit capabilities depending how the user configures SUNDIALS.

Temporary vectors were removed from preconditioner setup and solve routines for all packages. It is assumed that all necessary data for user-provided preconditioner operations will be allocated and stored in user-provided data structures.

The file include/sundials_fconfig.h was added. This file contains SUNDIALS type information for use in Fortran programs.

Added functions SUNDIALSGetVersion and SUNDIALSGetVersionNumber to get SUNDIALS release version information at runtime.

The build system was expanded to support many of the xSDK-compliant keys. The xSDK is a movement in scientific software to provide a foundation for the rapid and efficient production of high-quality, sustainable extreme-scale scientific applications. More information can be found at, https://xsdk.info.

In addition, numerous changes were made to the build system. Thes einclude the addition of separate BLAS_ENABLE and BLASLIBRARIES CMake variables, additional error checking during CMake configuration, minor bug fixes, and renaming CMake options to enable/disable examples for greater clarity and an added option to enable/disable Fortran 77 examples. These changes included changing ENABLE_EXAMPLES to ENABLE_EXAMPLES_C, changing CXX_ENABLE to EXAMPLES_ENABLE_CXX, changing F90_ENABLE to EXAMPLES_ENABKE_F90, and adding an EXAMPLES_ENABLE_F77 option.

A bug fix was done to add a missing prototype for IDASetMaxBacksIC in ida.h.

Corrections and additions were made to the examples, to installation-related files, and to the user documentation.

Changes in v1.3.0

Two additional NVECTOR implementations were added – one for Hypre (parallel) ParVector vectors, and one for PetSC vectors. These additions are accompanied by additions to various interface functions and to user documentation.

Each NVECTOR module now includes a function, `N_VGetVectorID`, that returns the NVECTOR module name.

An optional input function was added to set a maximum number of linesearch backtracks in the initial condition calculation, and four user-callable functions were added to support the use of LAPACK linear solvers in solving backward problems for adjoint sensitivity analysis.

For each linear solver, the various solver performance counters are now initialized to 0 in both the solver specification function and in solver `linit` function. This ensures that these solver counters are initialized upon linear solver instantiation as well as at the beginning of the problem solution.

A bug in for-loop indices was fixed in `IDAAckpntAllocVectors`. A bug was fixed in the interpolation functions used in solving backward problems.

A memory leak was fixed in the banded preconditioner interface. In addition, updates were done to return integers from linear solver and preconditioner 'free' functions.

In interpolation routines for backward problems, added logic to bypass sensitivity interpolation if input sensitivity argument is NULL.

The Krylov linear solver Bi-CGstab was enhanced by removing a redundant dot product. Various additions and corrections were made to the interfaces to the sparse solvers KLU and SuperLU_MT, including support for CSR format when using KLU.

New examples were added for use of the openMP vector and for use of sparse direct solvers within sensitivity integrations.

Minor corrections and additions were made to the IDAS solver, to the examples, to installation-related files, and to the user documentation.

Changes in v1.2.0

Two major additions were made to the linear system solvers that are available for use with the IDAS solver. First, in the serial case, an interface to the sparse direct solver KLU was added. Second, an interface to SuperLU_MT, the multi-threaded version of SuperLU, was added as a thread-parallel

sparse direct solver option, to be used with the serial version of the NVECTOR module. As part of these additions, a sparse matrix (CSC format) structure was added to IDAS.

Otherwise, only relatively minor modifications were made to IDAS:

In `IDARootfind`, a minor bug was corrected, where the input array `rootdir` was ignored, and a line was added to break out of root-search loop if the initial interval size is below the tolerance `ttol`.

In `IDALapackBand`, the line `smu = MIN(N-1,mu+ml)` was changed to `smu = mu + ml` to correct an illegal input error for `DGBTRF/DGBTRS`.

An option was added in the case of Adjoint Sensitivity Analysis with dense or banded Jacobian: With a call to `IDADlsSetDenseJacFnBS` or `IDADlsSetBandJacFnBS`, the user can specify a user-supplied Jacobian function of type `IDADls***JacFnBS`, for the case where the backward problem depends on the forward sensitivities.

A minor bug was fixed regarding the testing of the input `tstop` on the first call to `IDASolve`.

For the Adjoint Sensitivity Analysis case in which the backward problem depends on the forward sensitivities, options have been added to allow for user-supplied `pset`, `psolve`, and `jtimes` functions.

In order to avoid possible name conflicts, the mathematical macro and function names `MIN`, `MAX`, `SQR`, `RAbs`, `RSqrt`, `RExp`, `RPowerI`, and `RPowerR` were changed to `SUNMIN`, `SUNMAX`, `SUNSQR`, `SUNRabs`, `SUNRsqrt`, `SUNRexp`, `SRpowerI`, and `SUNRpowerR`, respectively. These names occur in both the solver and in various example programs.

In the User Guide, a paragraph was added in Section 6.2.1 on `IDAAdjReInit`, and a paragraph was added in Section 6.2.9 on `IDAGetAdjY`.

Two new NVECTOR modules have been added for thread-parallel computing environments — one for openMP, denoted `NVECTOR_OPENMP`, and one for Pthreads, denoted `NVECTOR_PTHREADS`.

With this version of SUNDIALS, support and documentation of the Autotools mode of installation is being dropped, in favor of the CMake mode, which is considered more widely portable.

Changes in v1.1.0

One significant design change was made with this release: The problem size and its relatives, bandwidth parameters, related internal indices, pivot arrays, and the optional output `lsflag` have all been changed from type `int` to type `long int`, except for the problem size and bandwidths in user calls to routines specifying BLAS/LAPACK routines for the dense/band linear solvers. The function `NewIntArray` is replaced by a pair `NewIntArray/NewLintArray`, for `int` and `long int` arrays, respectively. In a minor change to the user interface, the type of the index `which` in IDAS was changed from `long int` to `int`.

Errors in the logic for the integration of backward problems were identified and fixed.

A large number of minor errors have been fixed. Among these are the following: A missing vector pointer setting was added in `IDASensLineSrch`. In `IDACompleteStep`, conditionals around lines loading a new column of three auxiliary divided difference arrays, for a possible order increase, were fixed. After the solver memory is created, it is set to zero before being filled. In each linear solver interface function, the linear solver memory is freed on an error return, and the `**Free` function now includes a line setting to NULL the main memory pointer to the linear solver memory. A memory leak was fixed in two of the `IDASp***Free` functions. In the rootfinding functions `IDARcheck1/IDARcheck2`, when an exact zero is found, the array `glo` of g values at the left endpoint is adjusted, instead of shifting the t location `tlo` slightly. In the installation files, we modified the treatment of the macro SUNDIALS_USE_GENERIC_MATH, so that the parameter GENERIC_MATH_LIB is either defined (with no value) or not defined.

1.2 Reading this User Guide

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by IDAS for the solution of initial value problems for systems of DAEs, continue with short descriptions of

preconditioning (§2.2) and rootfinding (§2.3), and then give an overview of the mathematical aspects of sensitivity analysis, both forward (§2.5) and adjoint (§2.6).

- The following chapter describes the structure of the SUNDIALS suite of solvers (§3.1) and the software organization of the IDAS solver (§3.2).
- Chapter 4 is the main usage document for IDAS for simulation applications. It includes a complete description of the user interface for the integration of DAE initial value problems. Readers that are not interested in using IDAS for sensitivity analysis can then skip the next two chapters.
- Chapter 5 describes the usage of IDAS for forward sensitivity analysis as an extension of its IVP integration capabilities. We begin with a skeleton of the user main program, with emphasis on the steps that are required in addition to those already described in Chapter 4. Following that we provide detailed descriptions of the user-callable interface routines specific to forward sensitivity analysis and of the additonal optional user-defined routines.
- Chapter 6 describes the usage of IDAS for adjoint sensitivity analysis. We begin by describing the IDAS checkpointing implementation for interpolation of the original IVP solution during integration of the adjoint system backward in time, and with an overview of a user's main program. Following that we provide complete descriptions of the user-callable interface routines for adjoint sensitivity analysis as well as descriptions of the required additional user-defined routines.
- Chapter 7 gives a brief overview of the generic NVECTOR module shared amongst the various components of SUNDIALS, as well as details on the NVECTOR implementations provided with SUNDIALS.
- Chapter 10 describes the specifications of linear solver modules as supplied by the user.
- Chapter 11 describes in detail the generic linear solvers shared by all SUNDIALS solvers.
- Finally, in the appendices, we provide detailed instructions for the installation of IDAS, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from IDAS functions (Appendix B).

The reader should be aware of the following notational conventions in this user guide: program listings and identifiers (such as `IDAInit`) within textual explanations appear in typewriter type style; fields in C structures (such as *content*) appear in italics; and packages or modules, such as IDADENSE, are written in all capitals. Usage and installation instructions that constitute important warnings are marked with a triangular symbol in the margin.

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Chapter 2

Mathematical Considerations

IDAS solves the initial-value problem (IVP) for a DAE system of the general form

$$F(t, y, \dot{y}) = 0\,, \quad y(t_0) = y_0\,,\ \dot{y}(t_0) = \dot{y}_0\,, \tag{2.1}$$

where y, $\dot{y}$, and F are vectors in $\mathbf{R}^N$, t is the independent variable, $\dot{y} = dy/dt$, and initial values y_0, $\dot{y}_0$ are given. (Often t is time, but it certainly need not be.)

Additionally, if (2.1) depends on some parameters $p \in \mathbf{R}^{N_p}$, i.e.

$$\begin{aligned} &F(t, y, \dot{y}, p) = 0 \\ &y(t_0) = y_0(p)\,,\ \dot{y}(t_0) = \dot{y}_0(p)\,, \end{aligned} \tag{2.2}$$

IDAS can also compute first order derivative information, performing either *forward sensitivity analysis* or *adjoint sensitivity analysis*. In the first case, IDAS computes the sensitivities of the solution with respect to the parameters p, while in the second case, IDAS computes the gradient of a *derived function* with respect to the parameters p.

2.1 IVP solution

Prior to integrating a DAE initial-value problem, an important requirement is that the pair of vectors y_0 and $\dot{y}_0$ are both initialized to satisfy the DAE residual $F(t_0, y_0, \dot{y}_0) = 0$. For a class of problems that includes so-called semi-explicit index-one systems, IDAS provides a routine that computes consistent initial conditions from a user's initial guess [6]. For this, the user must identify sub-vectors of y (not necessarily contiguous), denoted y_d and y_a, which are its differential and algebraic parts, respectively, such that F depends on $\dot{y}_d$ but not on any components of $\dot{y}_a$. The assumption that the system is "index one" means that for a given t and y_d, the system $F(t, y, \dot{y}) = 0$ defines y_a uniquely. In this case, a solver within IDAS computes y_a and $\dot{y}_d$ at $t = t_0$, given y_d and an initial guess for y_a. A second available option with this solver also computes all of $y(t_0)$ given $\dot{y}(t_0)$; this is intended mainly for quasi-steady-state problems, where $\dot{y}(t_0) = 0$ is given. In both cases, IDAS solves the system $F(t_0, y_0, \dot{y}_0) = 0$ for the unknown components of y_0 and $\dot{y}_0$, using Newton iteration augmented with a line search global strategy. In doing this, it makes use of the existing machinery that is to be used for solving the linear systems during the integration, in combination with certain tricks involving the step size (which is set artificially for this calculation). For problems that do not fall into either of these categories, the user is responsible for passing consistent values, or risks failure in the numerical integration.

The integration method used in IDAS is the variable-order, variable-coefficient BDF (Backward Differentiation Formula), in fixed-leading-coefficient form [3]. The method order ranges from 1 to 5, with the BDF of order q given by the multistep formula

$$\sum_{i=0}^{q} \alpha_{n,i} y_{n-i} = h_n \dot{y}_n\,, \tag{2.3}$$

where y_n and $\dot{y}_n$ are the computed approximations to $y(t_n)$ and $\dot{y}(t_n)$, respectively, and the step size is $h_n = t_n - t_{n-1}$. The coefficients $\alpha_{n,i}$ are uniquely determined by the order q, and the history of the step sizes. The application of the BDF (2.3) to the DAE system (2.1) results in a nonlinear algebraic system to be solved at each step:

$$G(y_n) \equiv F\left(t_n,\, y_n,\, h_n^{-1} \sum_{i=0}^{q} \alpha_{n,i} y_{n-i}\right) = 0\,. \tag{2.4}$$

Regardless of the method options, the solution of the nonlinear system (2.4) is accomplished with some form of Newton iteration. This leads to a linear system for each Newton correction, of the form

$$J[y_{n(m+1)} - y_{n(m)}] = -G(y_{n(m)})\,, \tag{2.5}$$

where $y_{n(m)}$ is the m-th approximation to y_n. Here J is some approximation to the system Jacobian

$$J = \frac{\partial G}{\partial y} = \frac{\partial F}{\partial y} + \alpha \frac{\partial F}{\partial \dot{y}}\,, \tag{2.6}$$

where $\alpha = \alpha_{n,0}/h_n$. The scalar α changes whenever the step size or method order changes.

For the solution of the linear systems within the Newton corrections, IDAS provides several choices, including the option of an user-supplied linear solver module. The linear solver modules distributed with SUNDIALS are organized in three families, a *direct* family comprising direct linear solvers for dense or banded matrices, a *sparse* family comprising direct linear solvers for matrices stored in compressed-sparse-column format, and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, using either an internal implementation or a Blas/Lapack implementation (serial or threaded vector modules only),
- band direct solvers, using either an internal implementation or a Blas/Lapack implementation (serial or threaded vector modules only),
- sparse direct solver interfaces, using either the KLU sparse solver library [14, 1], or the thread-enabled SuperLU_MT sparse solver library [28, 15, 2] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SuperLU_MT packages independent of IDAS],
- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver without restarts,
- SPBCGS, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver, or
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver.

For large stiff systems, where direct methods are not feasible, the combination of a BDF integrator and any of the preconditioned Krylov methods (SPGMR, SPBCGS, or SPTFQMR) yields a powerful tool because it combines established methods for stiff integration, nonlinear iteration, and Krylov (linear) iteration with a problem-specific treatment of the dominant source of stiffness, in the form of the user-supplied preconditioner matrix [4]. For the *spils* linear solvers, preconditioning is allowed only on the left (see §2.2). Note that the direct linear solvers (dense, band, and sparse) can only be used with serial or threaded vector representations.

In the process of controlling errors at various levels, IDAS uses a weighted root-mean-square norm, denoted $\|\cdot\|_{\mathrm{WRMS}}$, for all error-like quantities. The multiplicative weights used are based on the current solution and on the relative and absolute tolerances input by the user, namely

$$W_i = 1/[\mathrm{RTOL} \cdot |y_i| + \mathrm{ATOL}_i]\,. \tag{2.7}$$

Because $1/W_i$ represents a tolerance in the component y_i, a vector whose norm is 1 is regarded as "small". For brevity, we will usually drop the subscript WRMS on norms in what follows.

In the case of a direct linear solver (dense, band, or sparse), the nonlinear iteration (2.5) is a Modified Newton iteration, in that the Jacobian J is fixed (and usually out of date), with a coefficient $\bar{\alpha}$ in place of α in J. When using one of the Krylov methods SPGMR, SPBCGS, or SPTFQMR as the linear solver, the iteration is an Inexact Newton iteration, using the current Jacobian (through matrix-free products Jv), in which the linear residual $J\Delta y + G$ is nonzero but controlled. The Jacobian matrix J (direct cases) or preconditioner matrix P (SPGMR/SPBCGS/SPTFQMR case) is updated when:

- starting the problem,
- the value $\bar{\alpha}$ at the last update is such that $\alpha/\bar{\alpha} < 3/5$ or $\alpha/\bar{\alpha} > 5/3$, or
- a non-fatal convergence failure occurred with an out-of-date J or P.

The above strategy balances the high cost of frequent matrix evaluations and preprocessing with the slow convergence due to infrequent updates. To reduce storage costs on an update, Jacobian information is always reevaluated from scratch.

The stopping test for the Newton iteration in IDAS ensures that the iteration error $y_n - y_{n(m)}$ is small relative to y itself. For this, we estimate the linear convergence rate at all iterations $m > 1$ as

$$R = \left(\frac{\delta_m}{\delta_1}\right)^{\frac{1}{m-1}} ,$$

where the $\delta_m = y_{n(m)} - y_{n(m-1)}$ is the correction at iteration $m = 1, 2, \ldots$. The Newton iteration is halted if $R > 0.9$. The convergence test at the m-th iteration is then

$$S\|\delta_m\| < 0.33 , \tag{2.8}$$

where $S = R/(R-1)$ whenever $m > 1$ and $R \le 0.9$. The user has the option of changing the constant in the convergence test from its default value of 0.33. The quantity S is set to $S = 20$ initially and whenever J or P is updated, and it is reset to $S = 100$ on a step with $\alpha \neq \bar{\alpha}$. Note that at $m = 1$, the convergence test (2.8) uses an old value for S. Therefore, at the first Newton iteration, we make an additional test and stop the iteration if $\|\delta_1\| < 0.33 \cdot 10^{-4}$ (since such a δ_1 is probably just noise and therefore not appropriate for use in evaluating R). We allow only a small number (default value 4) of Newton iterations. If convergence fails with J or P current, we are forced to reduce the step size h_n, and we replace h_n by $h_n/4$. The integration is halted after a preset number (default value 10) of convergence failures. Both the maximum allowable Newton iterations and the maximum nonlinear convergence failures can be changed by the user from their default values.

When SPGMR, SPBCGS, or SPTFQMR is used to solve the linear system, to minimize the effect of linear iteration errors on the nonlinear and local integration error controls, we require the preconditioned linear residual to be small relative to the allowed error in the Newton iteration, i.e., $\|P^{-1}(Jx + G)\| < 0.05 \cdot 0.33$. The safety factor 0.05 can be changed by the user.

In the direct linear solver cases, the Jacobian J defined in (2.6) can be either supplied by the user or have IDAS compute one internally by difference quotients. In the latter case, we use the approximation

$$\begin{aligned} J_{ij} &= [F_i(t, y + \sigma_j e_j, \dot{y} + \alpha\sigma_j e_j) - F_i(t, y, \dot{y})]/\sigma_j , \text{ with} \\ \sigma_j &= \sqrt{U} \max\{|y_j|, |h\dot{y}_j|, 1/W_j\} \operatorname{sign}(h\dot{y}_j) , \end{aligned}$$

where U is the unit roundoff, h is the current step size, and W_j is the error weight for the component y_j defined by (2.7). In the SPGMR/SPBCGS/SPTFQMR case, if a routine for Jv is not supplied, such products are approximated by

$$Jv = [F(t, y + \sigma v, \dot{y} + \alpha\sigma v) - F(t, y, \dot{y})]/\sigma ,$$

where the increment σ is $1/\|v\|$. As an option, the user can specify a constant factor that is inserted into this expression for σ.

We note that with the sparse direct solvers, the Jacobian *must* be supplied by a user routine in compressed-sparse-column format.

During the course of integrating the system, IDAS computes an estimate of the local truncation error, LTE, at the n-th time step, and requires this to satisfy the inequality

$$\|\text{LTE}\|_{\text{WRMS}} \leq 1\,.$$

Asymptotically, LTE varies as h^{q+1} at step size h and order q, as does the predictor-corrector difference $\Delta_n \equiv y_n - y_{n(0)}$. Thus there is a constant C such that

$$\text{LTE} = C\Delta_n + O(h^{q+2})\,,$$

and so the norm of LTE is estimated as $|C| \cdot \|\Delta_n\|$. In addition, IDAS requires that the error in the associated polynomial interpolant over the current step be bounded by 1 in norm. The leading term of the norm of this error is bounded by $\bar{C}\|\Delta_n\|$ for another constant $\bar{C}$. Thus the local error test in IDAS is

$$\max\{|C|, \bar{C}\}\|\Delta_n\| \leq 1\,. \tag{2.9}$$

A user option is available by which the algebraic components of the error vector are omitted from the test (2.9), if these have been so identified.

In IDAS, the local error test is tightly coupled with the logic for selecting the step size and order. First, there is an initial phase that is treated specially; for the first few steps, the step size is doubled and the order raised (from its initial value of 1) on every step, until (a) the local error test (2.9) fails, (b) the order is reduced (by the rules given below), or (c) the order reaches 5 (the maximum). For step and order selection on the general step, IDAS uses a different set of local error estimates, based on the asymptotic behavior of the local error in the case of fixed step sizes. At each of the orders q' equal to q, $q-1$ (if $q > 1$), $q-2$ (if $q > 2$), or $q+1$ (if $q < 5$), there are constants $C(q')$ such that the norm of the local truncation error at order q' satisfies

$$\text{LTE}(q') = C(q')\|\phi(q'+1)\| + O(h^{q'+2})\,,$$

where $\phi(k)$ is a modified divided difference of order k that is retained by IDAS (and behaves asymptotically as h^k). Thus the local truncation errors are estimated as $\text{ELTE}(q') = C(q')\|\phi(q'+1)\|$ to select step sizes. But the choice of order in IDAS is based on the requirement that the scaled derivative norms, $\|h^k y^{(k)}\|$, are monotonically decreasing with k, for k near q. These norms are again estimated using the $\phi(k)$, and in fact

$$\|h^{q'+1}y^{(q'+1)}\| \approx T(q') \equiv (q'+1)\text{ELTE}(q')\,.$$

The step/order selection begins with a test for monotonicity that is made even *before* the local error test is performed. Namely, the order is reset to $q' = q-1$ if (a) $q = 2$ and $T(1) \leq T(2)/2$, or (b) $q > 2$ and $\max\{T(q-1), T(q-2)\} \leq T(q)$; otherwise $q' = q$. Next the local error test (2.9) is performed, and if it fails, the step is redone at order $q \leftarrow q'$ and a new step size h'. The latter is based on the h^{q+1} asymptotic behavior of $\text{ELTE}(q)$, and, with safety factors, is given by

$$\eta = h'/h = 0.9/[2\,\text{ELTE}(q)]^{1/(q+1)}\,.$$

The value of η is adjusted so that $0.25 \leq \eta \leq 0.9$ before setting $h \leftarrow h' = \eta h$. If the local error test fails a second time, IDAS uses $\eta = 0.25$, and on the third and subsequent failures it uses $q = 1$ and $\eta = 0.25$. After 10 failures, IDAS returns with a give-up message.

As soon as the local error test has passed, the step and order for the next step may be adjusted. No such change is made if $q' = q-1$ from the prior test, if $q = 5$, or if q was increased on the previous step. Otherwise, if the last $q+1$ steps were taken at a constant order $q < 5$ and a constant step size, IDAS considers raising the order to $q+1$. The logic is as follows: (a) If $q = 1$, then reset $q = 2$ if $T(2) < T(1)/2$. (b) If $q > 1$ then

- reset $q \leftarrow q-1$ if $T(q-1) \leq \min\{T(q), T(q+1)\}$;

- else reset $q \leftarrow q+1$ if $T(q+1) < T(q)$;
- leave q unchanged otherwise [then $T(q-1) > T(q) \leq T(q+1)$].

In any case, the new step size h' is set much as before:

$$\eta = h'/h = 1/[2\,\mathrm{ELTE}(q)]^{1/(q+1)}\,.$$

The value of η is adjusted such that (a) if $\eta > 2$, η is reset to 2; (b) if $\eta \leq 1$, η is restricted to $0.5 \leq \eta \leq 0.9$; and (c) if $1 < \eta < 2$ we use $\eta = 1$. Finally h is reset to $h' = \eta h$. Thus we do not increase the step size unless it can be doubled. See [3] for details.

IDAS permits the user to impose optional inequality constraints on individual components of the solution vector y. Any of the following four constraints can be imposed: $y_i > 0$, $y_i < 0$, $y_i \geq 0$, or $y_i \leq 0$. The constraint satisfaction is tested after a successful nonlinear system solution. If any constraint fails, we declare a convergence failure of the Newton iteration and reduce the step size. Rather than cutting the step size by some arbitrary factor, IDAS estimates a new step size h' using a linear approximation of the components in y that failed the constraint test (including a safety factor of 0.9 to cover the strict inequality case). These additional constraints are also imposed during the calculation of consistent initial conditions.

Normally, IDAS takes steps until a user-defined output value $t = t_{\mathrm{out}}$ is overtaken, and then computes $y(t_{\mathrm{out}})$ by interpolation. However, a "one step" mode option is available, where control returns to the calling program after each step. There are also options to force IDAS not to integrate past a given stopping point $t = t_{\mathrm{stop}}$.

2.2 Preconditioning

When using a Newton method to solve the nonlinear system (2.5), IDAS makes repeated use of a linear solver to solve linear systems of the form $J\Delta y = -G$. If this linear system solve is done with one of the scaled preconditioned iterative linear solvers, these solvers are rarely successful if used without preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system $Ax = b$ can be preconditioned on the left, on the right, or on both sides. The Krylov method is then applied to a system with the matrix $P^{-1}A$, or AP^{-1}, or $P_L^{-1}AP_R^{-1}$, instead of A. However, within IDAS, preconditioning is allowed *only* on the left, so that the iterative method is applied to systems $(P^{-1}J)\Delta y = -P^{-1}G$. Left preconditioning is required to make the norm of the linear residual in the Newton iteration meaningful; in general, $\|J\Delta y + G\|$ is meaningless, since the weights used in the WRMS-norm correspond to y.

In order to improve the convergence of the Krylov iteration, the preconditioner matrix P should in some sense approximate the system matrix A. Yet at the same time, in order to be cost-effective, the matrix P should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [4] for an extensive study of preconditioners for reaction-transport systems).

Typical preconditioners used with IDAS are based on approximations to the Newton iteration matrix of the systems involved; in other words, $P \approx \frac{\partial F}{\partial y} + \alpha\frac{\partial F}{\partial \dot{y}}$, where α is a scalar inversely proportional to the integration step size h. Because the Krylov iteration occurs within a Newton iteration and further also within a time integration, and since each of these iterations has its own test for convergence, the preconditioner may use a very crude approximation, as long as it captures the dominant numerical feature(s) of the system. We have found that the combination of a preconditioner with the Newton-Krylov iteration, using even a fairly poor approximation to the Jacobian, can be surprisingly superior to using the same matrix without Krylov acceleration (i.e., a modified Newton iteration), as well as to using the Newton-Krylov method with no preconditioning.

2.3 Rootfinding

The IDAS solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (2.1), IDAS can also find the roots of a set of user-defined functions

$g_i(t, y, \dot{y})$ that depend on t, the solution vector $y = y(t)$, and its $t-$derivative $\dot{y}(t)$. The number of these root functions is arbitrary, and if more than one g_i is found to have a root in any given interval, the various root locations are found and reported in the order that they occur on the t axis, in the direction of integration.

Generally, this rootfinding feature finds only roots of odd multiplicity, corresponding to changes in sign of $g_i(t, y(t), \dot{y}(t))$, denoted $g_i(t)$ for short. If a user root function has a root of even multiplicity (no sign change), it will probably be missed by IDAS. If such a root is desired, the user should reformulate the root function so that it changes sign at the desired root.

The basic scheme used is to check for sign changes of any $g_i(t)$ over each time step taken, and then (when a sign change is found) to home in on the root (or roots) with a modified secant method [19]. In addition, each time g is computed, IDAS checks to see if $g_i(t) = 0$ exactly, and if so it reports this as a root. However, if an exact zero of any g_i is found at a point t, IDAS computes g at $t + \delta$ for a small increment δ, slightly further in the direction of integration, and if any $g_i(t + \delta) = 0$ also, IDAS stops and reports an error. This way, each time IDAS takes a time step, it is guaranteed that the values of all g_i are nonzero at some past value of t, beyond which a search for roots is to be done.

At any given time in the course of the time-stepping, after suitable checking and adjusting has been done, IDAS has an interval $(t_{lo}, t_{hi}]$ in which roots of the $g_i(t)$ are to be sought, such that t_{hi} is further ahead in the direction of integration, and all $g_i(t_{lo}) \neq 0$. The endpoint t_{hi} is either t_n, the end of the time step last taken, or the next requested output time t_{out} if this comes sooner. The endpoint t_{lo} is either t_{n-1}, or the last output time t_{out} (if this occurred within the last step), or the last root location (if a root was just located within this step), possibly adjusted slightly toward t_n if an exact zero was found. The algorithm checks g at t_{hi} for zeros and for sign changes in (t_{lo}, t_{hi}). If no sign changes are found, then either a root is reported (if some $g_i(t_{hi}) = 0$) or we proceed to the next time interval (starting at t_{hi}). If one or more sign changes were found, then a loop is entered to locate the root to within a rather tight tolerance, given by

$$\tau = 100 * U * (|t_n| + |h|) \quad (U = \text{unit roundoff}) \ .$$

Whenever sign changes are seen in two or more root functions, the one deemed most likely to have its root occur first is the one with the largest value of $|g_i(t_{hi})|/|g_i(t_{hi}) - g_i(t_{lo})|$, corresponding to the closest to t_{lo} of the secant method values. At each pass through the loop, a new value t_{mid} is set, strictly within the search interval, and the values of $g_i(t_{mid})$ are checked. Then either t_{lo} or t_{hi} is reset to t_{mid} according to which subinterval is found to have the sign change. If there is none in (t_{lo}, t_{mid}) but some $g_i(t_{mid}) = 0$, then that root is reported. The loop continues until $|t_{hi} - t_{lo}| < \tau$, and then the reported root location is t_{hi}.

In the loop to locate the root of $g_i(t)$, the formula for t_{mid} is

$$t_{mid} = t_{hi} - (t_{hi} - t_{lo}) g_i(t_{hi}) / [g_i(t_{hi}) - \alpha g_i(t_{lo})] \ ,$$

where α a weight parameter. On the first two passes through the loop, α is set to 1, making t_{mid} the secant method value. Thereafter, α is reset according to the side of the subinterval (low vs high, i.e. toward t_{lo} vs toward t_{hi}) in which the sign change was found in the previous two passes. If the two sides were opposite, α is set to 1. If the two sides were the same, α is halved (if on the low side) or doubled (if on the high side). The value of t_{mid} is closer to t_{lo} when $\alpha < 1$ and closer to t_{hi} when $\alpha > 1$. If the above value of t_{mid} is within $\tau/2$ of t_{lo} or t_{hi}, it is adjusted inward, such that its fractional distance from the endpoint (relative to the interval size) is between .1 and .5 (.5 being the midpoint), and the actual distance from the endpoint is at least $\tau/2$.

2.4 Pure quadrature integration

In many applications, and most notably during the backward integration phase of an adjoint sensitivity analysis run (see §2.6) it is of interest to compute integral quantities of the form

$$z(t) = \int_{t_0}^{t} q(\tau, y(\tau), \dot{y}(\tau), p) \, d\tau \ . \tag{2.10}$$

The most effective approach to compute $z(t)$ is to extend the original problem with the additional ODEs (obtained by applying Leibnitz's differentiation rule):

$$\dot{z} = q(t, y, \dot{y}, p)\,, \quad z(t_0) = 0\,. \tag{2.11}$$

Note that this is equivalent to using a quadrature method based on the underlying linear multistep polynomial representation for $y(t)$.

This can be done at the "user level" by simply exposing to IDAS the extended DAE system (2.2)+(2.10). However, in the context of an implicit integration solver, this approach is not desirable since the nonlinear solver module will require the Jacobian (or Jacobian-vector product) of this extended DAE. Moreover, since the additional states z do not enter the right-hand side of the ODE (2.10) and therefore the residual of the extended DAE system does not depend on z, it is much more efficient to treat the ODE system (2.10) separately from the original DAE system (2.2) by "taking out" the additional states z from the nonlinear system (2.4) that must be solved in the correction step of the LMM. Instead, "corrected" values z_n are computed explicitly as

$$z_n = \frac{1}{\alpha_{n,0}} \left(h_n q(t_n, y_n, \dot{y}_n, p) - \sum_{i=1}^{q} \alpha_{n,i} z_{n-i} \right)\,,$$

once the new approximation y_n is available.

The quadrature variables z can be optionally included in the error test, in which case corresponding relative and absolute tolerances must be provided.

2.5 Forward sensitivity analysis

Typically, the governing equations of complex, large-scale models depend on various parameters, through the right-hand side vector and/or through the vector of initial conditions, as in (2.2). In addition to numerically solving the DAEs, it may be desirable to determine the sensitivity of the results with respect to the model parameters. Such sensitivity information can be used to estimate which parameters are most influential in affecting the behavior of the simulation or to evaluate optimization gradients (in the setting of dynamic optimization, parameter estimation, optimal control, etc.).

The *solution sensitivity* with respect to the model parameter p_i is defined as the vector $s_i(t) = \partial y(t)/\partial p_i$ and satisfies the following *forward sensitivity equations* (or *sensitivity equations* for short):

$$\begin{aligned} &\frac{\partial F}{\partial y} s_i + \frac{\partial F}{\partial \dot{y}} \dot{s}_i + \frac{\partial F}{\partial p_i} = 0 \\ &s_i(t_0) = \frac{\partial y_0(p)}{\partial p_i}\,, \;\; \dot{s}_i(t_0) = \frac{\partial \dot{y}_0(p)}{\partial p_i}\,, \end{aligned} \tag{2.12}$$

obtained by applying the chain rule of differentiation to the original DAEs (2.2).

When performing forward sensitivity analysis, IDAS carries out the time integration of the combined system, (2.2) and (2.12), by viewing it as a DAE system of size $N(N_s + 1)$, where N_s is the number of model parameters p_i, with respect to which sensitivities are desired ($N_s \leq N_p$). However, major improvements in efficiency can be made by taking advantage of the special form of the sensitivity equations as linearizations of the original DAEs. In particular, the original DAE system and all sensitivity systems share the same Jacobian matrix J in (2.6).

The sensitivity equations are solved with the same linear multistep formula that was selected for the original DAEs and the same linear solver is used in the correction phase for both state and sensitivity variables. In addition, IDAS offers the option of including (*full error control*) or excluding (*partial error control*) the sensitivity variables from the local error test.

2.5.1 Forward sensitivity methods

In what follows we briefly describe three methods that have been proposed for the solution of the combined DAE and sensitivity system for the vector $\hat{y} = [y, s_1, \ldots, s_{N_s}]$.

- *Staggered Direct* In this approach [11], the nonlinear system (2.4) is first solved and, once an acceptable numerical solution is obtained, the sensitivity variables at the new step are found by directly solving (2.12) after the BDF discretization is used to eliminate $\dot{s}_i$. Although the system matrix of the above linear system is based on exactly the same information as the matrix J in (2.6), it must be updated and factored at every step of the integration, in contrast to an evaluation of J which is updated only occasionally. For problems with many parameters (relative to the problem size), the staggered direct method can outperform the methods described below [27]. However, the computational cost associated with matrix updates and factorizations makes this method unattractive for problems with many more states than parameters (such as those arising from semidiscretization of PDEs) and is therefore not implemented in IDAS.

- *Simultaneous Corrector* In this method [29], the discretization is applied simultaneously to both the original equations (2.2) and the sensitivity systems (2.12) resulting in an "extended" nonlinear system $\hat{G}(\hat{y}_n) = 0$ where $\hat{y}_n = [y_n, \ldots, s_i, \ldots]$. This combined nonlinear system can be solved using a modified Newton method as in (2.5) by solving the corrector equation

$$\hat{J}[\hat{y}_{n(m+1)} - \hat{y}_{n(m)}] = -\hat{G}(\hat{y}_{n(m)}) \tag{2.13}$$

  at each iteration, where

$$\hat{J} = \begin{bmatrix} J & & & & \\ J_1 & J & & & \\ J_2 & 0 & J & & \\ \vdots & \vdots & \ddots & \ddots & \\ J_{N_s} & 0 & \ldots & 0 & J \end{bmatrix},$$

  J is defined as in (2.6), and $J_i = (\partial/\partial y)\,[F_y s_i + F_{\dot{y}} \dot{s}_i + F_{p_i}]$. It can be shown that 2-step quadratic convergence can be retained by using only the block-diagonal portion of $\hat{J}$ in the corrector equation (2.13). This results in a decoupling that allows the reuse of J without additional matrix factorizations. However, the sum $F_y s_i + F_{\dot{y}} \dot{s}_i + F_{p_i}$ must still be reevaluated at each step of the iterative process (2.13) to update the sensitivity portions of the residual $\hat{G}$.

- *Staggered corrector* In this approach [16], as in the staggered direct method, the nonlinear system (2.4) is solved first using the Newton iteration (2.5). Then, for each sensitivity vector $\xi \equiv s_i$, a separate Newton iteration is used to solve the sensitivity system (2.12):

$$\begin{aligned} &J[\xi_{n(m+1)} - \xi_{n(m)}] = \\ &- \left[F_y(t_n, y_n, \dot{y}_n)\xi_{n(m)} + F_{\dot{y}}(t_n, y_n, \dot{y}_n) \cdot h_n^{-1} \left(\alpha_{n,0}\xi_{n(m)} + \sum_{i=1}^{q} \alpha_{n,i}\xi_{n-i} \right) + F_{p_i}(t_n, y_n, \dot{y}_n) \right]. \end{aligned} \tag{2.14}$$

  In other words, a modified Newton iteration is used to solve a linear system. In this approach, the matrices $\partial F/\partial y$, $\partial F/\partial \dot{y}$ and vectors $\partial F/\partial p_i$ need be updated only once per integration step, after the state correction phase (2.5) has converged.

IDAS implements both the simultaneous corrector method and the staggered corrector method.

An important observation is that the staggered corrector method, combined with a Krylov linear solver, effectively results in a staggered direct method. Indeed, the Krylov solver requires only the action of the matrix J on a vector and this can be provided with the current Jacobian information. Therefore, the modified Newton procedure (2.14) will theoretically converge after one iteration.

2.5.2 Selection of the absolute tolerances for sensitivity variables

If the sensitivities are included in the error test, IDAS provides an automated estimation of absolute tolerances for the sensitivity variables based on the absolute tolerance for the corresponding state variable. The relative tolerance for sensitivity variables is set to be the same as for the state variables.

The selection of absolute tolerances for the sensitivity variables is based on the observation that the sensitivity vector s_i will have units of $[y]/[p_i]$. With this, the absolute tolerance for the j-th component of the sensitivity vector s_i is set to $\text{ATOL}_j/|\bar{p}_i|$, where ATOL_j are the absolute tolerances for the state variables and $\bar{p}$ is a vector of scaling factors that are dimensionally consistent with the model parameters p and give an indication of their order of magnitude. This choice of relative and absolute tolerances is equivalent to requiring that the weighted root-mean-square norm of the sensitivity vector s_i with weights based on s_i be the same as the weighted root-mean-square norm of the vector of scaled sensitivities $\bar{s}_i = |\bar{p}_i| s_i$ with weights based on the state variables (the scaled sensitivities $\bar{s}_i$ being dimensionally consistent with the state variables). However, this choice of tolerances for the s_i may be a poor one, and the user of IDAS can provide different values as an option.

2.5.3 Evaluation of the sensitivity right-hand side

There are several methods for evaluating the residual functions in the sensitivity systems (2.12): analytic evaluation, automatic differentiation, complex-step approximation, and finite differences (or directional derivatives). IDAS provides all the software hooks for implementing interfaces to automatic differentiation (AD) or complex-step approximation; future versions will include a generic interface to AD-generated functions. At the present time, besides the option for analytical sensitivity right-hand sides (user-provided), IDAS can evaluate these quantities using various finite difference-based approximations to evaluate the terms $(\partial F/\partial y)s_i + (\partial F/\partial \dot{y})\dot{s}_i$ and $(\partial F/\partial p_i)$, or using directional derivatives to evaluate $[(\partial F/\partial y)s_i + (\partial F/\partial \dot{y})\dot{s}_i + (\partial F/\partial p_i)]$. As is typical for finite differences, the proper choice of perturbations is a delicate matter. IDAS takes into account several problem-related features: the relative DAE error tolerance RTOL, the machine unit roundoff U, the scale factor $\bar{p}_i$, and the weighted root-mean-square norm of the sensitivity vector s_i.

Using central finite differences as an example, the two terms $(\partial F/\partial y)s_i + (\partial F/\partial \dot{y})\dot{s}_i$ and $\partial F/\partial p_i$ in (2.12) can be evaluated either separately:

$$\frac{\partial F}{\partial y}s_i + \frac{\partial F}{\partial \dot{y}}\dot{s}_i \approx \frac{F(t, y+\sigma_y s_i, \dot{y}+\sigma_y \dot{s}_i, p) - F(t, y-\sigma_y s_i, \dot{y}-\sigma_y \dot{s}_i, p)}{2\,\sigma_y}\,, \tag{2.15}$$

$$\frac{\partial F}{\partial p_i} \approx \frac{F(t, y, \dot{y}, p+\sigma_i e_i) - F(t, y, \dot{y}, p-\sigma_i e_i)}{2\,\sigma_i}\,, \tag{2.15'}$$

$$\sigma_i = |\bar{p}_i|\sqrt{\max(\text{RTOL}, U)}\,, \quad \sigma_y = \frac{1}{\max(1/\sigma_i, \|s_i\|_{\text{WRMS}}/|\bar{p}_i|)}\,,$$

or simultaneously:

$$\frac{\partial F}{\partial y}s_i + \frac{\partial F}{\partial \dot{y}}\dot{s}_i + \frac{\partial F}{\partial p_i} \approx \frac{F(t, y+\sigma s_i, \dot{y}+\sigma \dot{s}_i, p+\sigma e_i) - F(t, y-\sigma s_i, \dot{y}-\sigma \dot{s}_i, p-\sigma e_i)}{2\,\sigma}\,, \tag{2.16}$$

$$\sigma = \min(\sigma_i, \sigma_y)\,,$$

or by adaptively switching between (2.15)+(2.15') and (2.16), depending on the relative size of the two finite difference increments σ_i and σ_y. In the adaptive scheme, if $\rho = \max(\sigma_i/\sigma_y, \sigma_y/\sigma_i)$, we use separate evaluations if $\rho > \rho_{\max}$ (an input value), and simultaneous evaluations otherwise.

These procedures for choosing the perturbations (σ_i, σ_y, σ) and switching between derivative formulas have also been implemented for one-sided difference formulas. Forward finite differences can be applied to $(\partial F/\partial y)s_i + (\partial F/\partial \dot{y})\dot{s}_i$ and $\frac{\partial F}{\partial p_i}$ separately, or the single directional derivative formula

$$\frac{\partial F}{\partial y}s_i + \frac{\partial F}{\partial \dot{y}}\dot{s}_i + \frac{\partial F}{\partial p_i} \approx \frac{F(t, y+\sigma s_i, \dot{y}+\sigma \dot{s}_i, p+\sigma e_i) - F(t, y, \dot{y}, p)}{\sigma}$$

can be used. In IDAS, the default value of $\rho_{\max} = 0$ indicates the use of the second-order centered directional derivative formula (2.16) exclusively. Otherwise, the magnitude of $\rho_{\max}$ and its sign (positive or negative) indicates whether this switching is done with regard to (centered or forward) finite differences, respectively.

2.5.4 Quadratures depending on forward sensitivities

If pure quadrature variables are also included in the problem definition (see §2.4), IDAS does *not* carry their sensitivities automatically. Instead, we provide a more general feature through which integrals depending on both the states y of (2.2) and the state sensitivities s_i of (2.12) can be evaluated. In other words, IDAS provides support for computing integrals of the form:

$$\bar{z}(t) = \int_{t_0}^{t} \bar{q}(\tau, y(\tau), \dot{y}(\tau), s_1(\tau), \ldots, s_{N_p}(\tau), p)\, d\tau\,.$$

If the sensitivities of the quadrature variables z of (2.10) are desired, these can then be computed by using:

$$\bar{q}_i = q_y s_i + q_{\dot{y}} \dot{s}_i + q_{p_i}\,, \quad i = 1, \ldots, N_p\,,$$

as integrands for $\bar{z}$, where q_y, $q_{\dot{y}}$, and q_p are the partial derivatives of the integrand function q of (2.10).

As with the quadrature variables z, the new variables $\bar{z}$ are also excluded from any nonlinear solver phase and "corrected" values $\bar{z}_n$ are obtained through explicit formulas.

2.6 Adjoint sensitivity analysis

In the *forward sensitivity approach* described in the previous section, obtaining sensitivities with respect to N_s parameters is roughly equivalent to solving an DAE system of size $(1 + N_s)N$. This can become prohibitively expensive, especially for large-scale problems, if sensitivities with respect to many parameters are desired. In this situation, the *adjoint sensitivity method* is a very attractive alternative, provided that we do not need the solution sensitivities s_i, but rather the gradients with respect to model parameters of a relatively few derived functionals of the solution. In other words, if $y(t)$ is the solution of (2.2), we wish to evaluate the gradient dG/dp of

$$G(p) = \int_{t_0}^{T} g(t, y, p)dt\,, \tag{2.17}$$

or, alternatively, the gradient dg/dp of the function $g(t, y, p)$ at the final time $t = T$. The function g must be smooth enough that $\partial g/\partial y$ and $\partial g/\partial p$ exist and are bounded.

In what follows, we only sketch the analysis for the sensitivity problem for both G and g. For details on the derivation see [10].

2.6.1 Sensitivity of $G(p)$

We focus first on solving the sensitivity problem for $G(p)$ defined by (2.17). Introducing a Lagrange multiplier λ, we form the augmented objective function

$$I(p) = G(p) - \int_{t_0}^{T} \lambda^* F(t, y, \dot{y}, p)dt.$$

Since $F(t, y, \dot{y}, p) = 0$, the sensitivity of G with respect to p is

$$\frac{dG}{dp} = \frac{dI}{dp} = \int_{t_0}^{T} (g_p + g_y y_p)dt - \int_{t_0}^{T} \lambda^*(F_p + F_y y_p + F_{\dot{y}}\dot{y}_p)dt, \tag{2.18}$$

where subscripts on functions such as F or g are used to denote partial derivatives. By integration by parts, we have

$$\int_{t_0}^{T} \lambda^* F_{\dot{y}}\dot{y}_p dt = (\lambda^* F_{\dot{y}} y_p)|_{t_0}^{T} - \int_{t_0}^{T} (\lambda^* F_{\dot{y}})' y_p dt,$$

where $(\cdots)'$ denotes the $t-$derivative. Thus equation (2.18) becomes

$$\frac{dG}{dp} = \int_{t_0}^{T} (g_p - \lambda^* F_p)\, dt - \int_{t_0}^{T} \left[-g_y + \lambda^* F_y - (\lambda^* F_{\dot{y}})'\right] y_p dt - (\lambda^* F_{\dot{y}} y_p)|_{t_0}^{T}. \tag{2.19}$$

Now by requiring λ to satisfy

$$(\lambda^* F_{\dot{y}})' - \lambda^* F_y = -g_y, \tag{2.20}$$

we obtain

$$\frac{dG}{dp} = \int_{t_0}^{T} (g_p - \lambda^* F_p)\, dt - (\lambda^* F_{\dot{y}} y_p)|_{t_0}^{T}. \tag{2.21}$$

Note that y_p at $t = t_0$ is the sensitivity of the initial conditions with respect to p, which is easily obtained. To find the initial conditions (at $t = T$) for the adjoint system, we must take into consideration the structure of the DAE system.

For index-0 and index-1 DAE systems, we can simply take

$$\lambda^* F_{\dot{y}}|_{t=T} = 0, \tag{2.22}$$

yielding the sensitivity equation for dG/dp

$$\frac{dG}{dp} = \int_{t_0}^{T} (g_p - \lambda^* F_p)\, dt + (\lambda^* F_{\dot{y}} y_p)|_{t=t_0}. \tag{2.23}$$

This choice will not suffice for a Hessenberg index-2 DAE system. For a derivation of proper final conditions in such cases, see [10].

The first thing to notice about the adjoint system (2.20) is that there is no explicit specification of the parameters p; this implies that, once the solution λ is found, the formula (2.21) can then be used to find the gradient of G with respect to any of the parameters p. The second important remark is that the adjoint system (2.20) is a terminal value problem which depends on the solution $y(t)$ of the original IVP (2.2). Therefore, a procedure is needed for providing the states y obtained during a forward integration phase of (2.2) to IDAS during the backward integration phase of (2.20). The approach adopted in IDAS, based on *checkpointing*, is described in §2.6.3 below.

2.6.2 Sensitivity of $g(T, p)$

Now let us consider the computation of $dg/dp(T)$. From $dg/dp(T) = (d/dT)(dG/dp)$ and equation (2.21), we have

$$\frac{dg}{dp} = (g_p - \lambda^* F_p)(T) - \int_{t_0}^{T} \lambda_T^* F_p dt + (\lambda_T^* F_{\dot{y}} y_p)|_{t=t_0} - \frac{d(\lambda^* F_{\dot{y}} y_p)}{dT} \tag{2.24}$$

where λ_T denotes $\partial\lambda/\partial T$. For index-0 and index-1 DAEs, we obtain

$$\frac{d(\lambda^* F_{\dot{y}} y_p)|_{t=T}}{dT} = 0,$$

while for a Hessenberg index-2 DAE system we have

$$\frac{d(\lambda^* F_{\dot{y}} y_p)|_{t=T}}{dT} = -\left.\frac{d(g_{y^a}(CB)^{-1} f_p^2)}{dt}\right|_{t=T}.$$

The corresponding adjoint equations are

$$(\lambda_T^* F_{\dot{y}})' - \lambda_T^* F_y = 0. \tag{2.25}$$

For index-0 and index-1 DAEs (as shown above, the index-2 case is different), to find the boundary condition for this equation we write λ as $\lambda(t, T)$ because it depends on both t and T. Then

$$\lambda^*(T, T) F_{\dot{y}}|_{t=T} = 0.$$

Taking the total derivative, we obtain

$$(\lambda_t + \lambda_T)^*(T,T)F_{\dot{y}}|_{t=T} + \lambda^*(T,T)\frac{dF_{\dot{y}}}{dt}|_{t=T} = 0.$$

Since λ_t is just $\dot{\lambda}$, we have the boundary condition

$$(\lambda_T^* F_{\dot{y}})|_{t=T} = -\left[\lambda^*(T,T)\frac{dF_{\dot{y}}}{dt} + \dot{\lambda}^* F_{\dot{y}}\right]|_{t=T}.$$

For the index-one DAE case, the above relation and (2.20) yield

$$(\lambda_T^* F_{\dot{y}})|_{t=T} = [g_y - \lambda^* F_y]\,|_{t=T}. \tag{2.26}$$

For the regular implicit ODE case, $F_{\dot{y}}$ is invertible; thus we have $\lambda(T,T) = 0$, which leads to $\lambda_T(T) = -\dot{\lambda}(T)$. As with the final conditions for $\lambda(T)$ in (2.20), the above selection for $\lambda_T(T)$ is not sufficient for index-two Hessenberg DAEs (see [10] for details).

2.6.3 Checkpointing scheme

During the backward integration, the evaluation of the right-hand side of the adjoint system requires, at the current time, the states y which were computed during the forward integration phase. Since IDAS implements variable-step integration formulas, it is unlikely that the states will be available at the desired time and so some form of interpolation is needed. The IDAS implementation being also variable-order, it is possible that during the forward integration phase the order may be reduced as low as first order, which means that there may be points in time where only y and $\dot{y}$ are available. These requirements therefore limit the choices for possible interpolation schemes. IDAS implements two interpolation methods: a cubic Hermite interpolation algorithm and a variable-degree polynomial interpolation method which attempts to mimic the BDF interpolant for the forward integration.

However, especially for large-scale problems and long integration intervals, the number and size of the vectors y and $\dot{y}$ that would need to be stored make this approach computationally intractable. Thus, IDAS settles for a compromise between storage space and execution time by implementing a so-called *checkpointing scheme*. At the cost of at most one additional forward integration, this approach offers the best possible estimate of memory requirements for adjoint sensitivity analysis. To begin with, based on the problem size N and the available memory, the user decides on the number N_d of data pairs $(y,\ \dot{y})$ if cubic Hermite interpolation is selected, or on the number N_d of y vectors in the case of variable-degree polynomial interpolation, that can be kept in memory for the purpose of interpolation. Then, during the first forward integration stage, after every N_d integration steps a checkpoint is formed by saving enough information (either in memory or on disk) to allow for a hot restart, that is a restart which will exactly reproduce the forward integration. In order to avoid storing Jacobian-related data at each checkpoint, a reevaluation of the iteration matrix is forced before each checkpoint. At the end of this stage, we are left with N_c checkpoints, including one at t_0. During the backward integration stage, the adjoint variables are integrated backwards from T to t_0, going from one checkpoint to the previous one. The backward integration from checkpoint $i+1$ to checkpoint i is preceded by a forward integration from i to $i+1$ during which the N_d vectors y (and, if necessary $\dot{y}$) are generated and stored in memory for interpolation[1]

This approach transfers the uncertainty in the number of integration steps in the forward integration phase to uncertainty in the final number of checkpoints. However, N_c is much smaller than the number of steps taken during the forward integration, and there is no major penalty for writing/reading the checkpoint data to/from a temporary file. Note that, at the end of the first forward

[1]The degree of the interpolation polynomial is always that of the current BDF order for the forward interpolation at the first point to the right of the time at which the interpolated value is sought (unless too close to the i-th checkpoint, in which case it uses the BDF order at the right-most relevant point). However, because of the FLC BDF implementation (see §2.1), the resulting interpolation polynomial is only an approximation to the underlying BDF interpolant.

The Hermite cubic interpolation option is present because it was implemented chronologically first and it is also used by other adjoint solvers (e.g. DASPKADJOINT). The variable-degree polynomial is more memory-efficient (it requires only half of the memory storage of the cubic Hermite interpolation) and is more accurate.

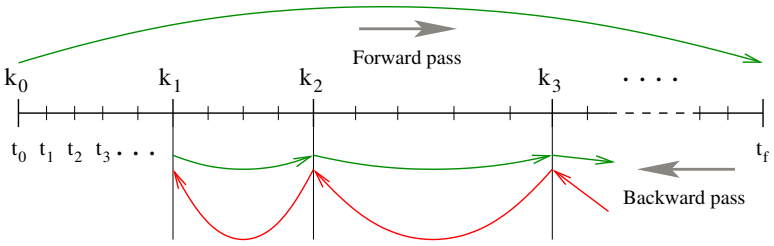


Figure 2.1: Illustration of the checkpointing algorithm for generation of the forward solution during the integration of the adjoint system.

integration stage, interpolation data are available from the last checkpoint to the end of the interval of integration. If no checkpoints are necessary (N_d is larger than the number of integration steps taken in the solution of (2.2)), the total cost of an adjoint sensitivity computation can be as low as one forward plus one backward integration. In addition, IDAS provides the capability of reusing a set of checkpoints for multiple backward integrations, thus allowing for efficient computation of gradients of several functionals (2.17).

Finally, we note that the adjoint sensitivity module in IDAS provides the necessary infrastructure to integrate backwards in time any DAE terminal value problem dependent on the solution of the IVP (2.2), including adjoint systems (2.20) or (2.25), as well as any other quadrature ODEs that may be needed in evaluating the integrals in (2.21). In particular, for DAE systems arising from semi-discretization of time-dependent PDEs, this feature allows for integration of either the discretized adjoint PDE system or the adjoint of the discretized PDE.

2.7 Second-order sensitivity analysis

In some applications (e.g., dynamically-constrained optimization) it may be desirable to compute second-order derivative information. Considering the DAE problem (2.2) and some model output functional[2] $g(y)$, the Hessian d^2g/dp^2 can be obtained in a forward sensitivity analysis setting as

$$\frac{d^2g}{dp^2} = \left(g_y \otimes I_{N_p}\right) y_{pp} + y_p^T g_{yy} y_p \,,$$

where $\otimes$ is the Kronecker product. The second-order sensitivities are solution of the matrix DAE system:

$$\left(F_{\dot{y}} \otimes I_{N_p}\right) \cdot \dot{y}_{pp} + \left(F_y \otimes I_{N_p}\right) \cdot y_{pp} + \left(I_N \otimes \dot{y}_p^T\right) \cdot \left(F_{\dot{y}\dot{y}} \dot{y}_p + F_{y\dot{y}} y_p\right) + \left(I_N \otimes y_p^T\right) \cdot \left(F_{y\dot{y}} \dot{y}_p + F_{yy} y_p\right) = 0$$

$$y_{pp}(t_0) = \frac{\partial^2 y_0}{\partial p^2} \,, \quad \dot{y}_{pp}(t_0) = \frac{\partial^2 \dot{y}_0}{\partial p^2} \,,$$

where y_p denotes the first-order sensitivity matrix, the solution of N_p systems (2.12), and y_{pp} is a third-order tensor. It is easy to see that, except for situations in which the number of parameters N_p is very small, the computational cost of this so-called *forward-over-forward* approach is exorbitant as it requires the solution of $N_p + N_p^2$ additional DAE systems of the same dimension as (2.2).

A much more efficient alternative is to compute Hessian-vector products using a so-called *forward-over-adjoint* approach. This method is based on using the same "trick" as the one used in computing gradients of pointwise functionals with the adjoint method, namely applying a formal directional forward derivation to the gradient of (2.21) (or the equivalent one for a pointwise functional $g(T, y(T))$).

[2] For the sake of simplifity in presentation, we do not include explicit dependencies of g on time t or parameters p. Moreover, we only consider the case in which the dependency of the original DAE (2.2) on the parameters p is through its initial conditions only. For details on the derivation in the general case, see [30].

With that, the cost of computing a full Hessian is roughly equivalent to the cost of computing the gradient with forward sensitivity analysis. However, Hessian-vector products can be cheaply computed with one additional adjoint solve.

As an illustration[3], consider the ODE problem

$$\dot{y} = f(t, y)\,, \quad y(t_0) = y_0(p)\,,$$

depending on some parameters p through the initial conditions only and consider the model functional output $G(p) = \int_{t_0}^{t_f} g(t, y)\, dt$. It can be shown that the product between the Hessian of G (with respect to the parameters p) and some vector u can be computed as

$$\frac{\partial^2 G}{\partial p^2} u = \left[\left(\lambda^T \otimes I_{N_p} \right) y_{pp} u + y_p^T \mu \right]_{t=t_0}\,,$$

where λ and μ are solutions of

$$\begin{aligned} -\dot{\mu} &= f_y^T \mu + \left(\lambda^T \otimes I_n \right) f_{yy} s\,; \quad \mu(t_f) = 0 \\ -\dot{\lambda} &= f_y^T \lambda + g_y^T\,; \quad \lambda(t_f) = 0 \\ \dot{s} &= f_y s\,; \quad s(t_0) = y_{0p} u. \end{aligned} \tag{2.27}$$

In the above equation, $s = y_p u$ is a linear combination of the columns of the sensitivity matrix y_p. The *forward-over-adjoint* approach hinges crucially on the fact that s can be computed at the cost of a forward sensitivity analysis with respect to a single parameter (the last ODE problem above) which is possible due to the linearity of the forward sensitivity equations (2.12).

Therefore (and this is also valid for the DAE case), the cost of computing the Hessian-vector product is roughly that of two forward and two backward integrations of a system of DAEs of size N. For more details, including the corresponding formulas for a pointwise model functional output, see the work by Ozyurt and Barton [30] who discuss this problem for ODE initial value problems. As far as we know, there is no published equivalent work on DAE problems. However, the derivations given in [30] for ODE problems can be extended to DAEs with some careful consideration given to the derivation of proper final conditions on the adjoint systems, following the ideas presented in [10].

To allow the *foward-over-adjoint* approach described above, IDAS provides support for:

- the integration of multiple backward problems depending on the same underlying forward problem (2.2), and
- the integration of backward problems and computation of backward quadratures depending on both the states y and forward sensitivities (for this particular application, s) of the original problem (2.2).

[3]The derivation for the general DAE case is too involved for the purposes of this discussion.

Chapter 3

Code Organization

3.1 SUNDIALS organization

The family of solvers referred to as SUNDIALS consists of the solvers CVODE and ARKODE (for ODE systems), KINSOL (for nonlinear algebraic systems), and IDA (for differential-algebraic systems). In addition, SUNDIALS also includes variants of CVODE and IDA with sensitivity analysis capabilities (using either forward or adjoint methods), called CVODES and IDAS, respectively.

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Fig. 3.1). The following is a list of the solver packages presently available, and the basic functionality of each:

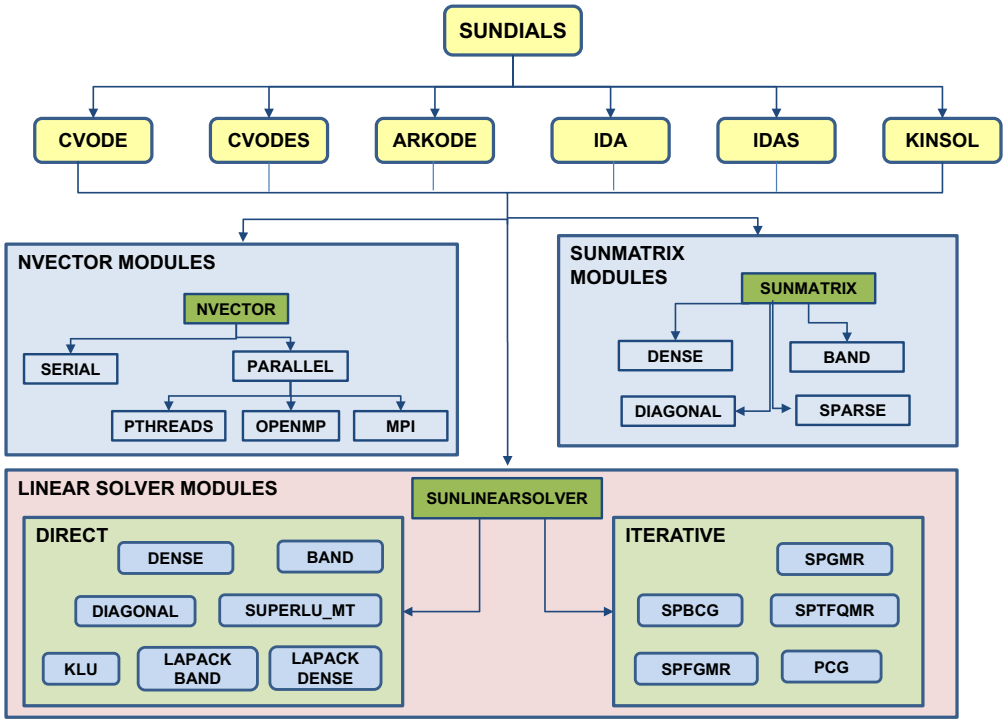
- CVODE, a solver for stiff and nonstiff ODE systems $dy/dt = f(t, y)$ based on Adams and BDF methods;
- CVODES, a solver for stiff and nonstiff ODE systems with sensitivity analysis capabilities;
- ARKODE, a solver for ODE systems $M dy/dt = f_E(t, y) + f_I(t, y)$ based on additive Runge-Kutta methods;
- IDA, a solver for differential-algebraic systems $F(t, y, \dot{y}) = 0$ based on BDF methods;
- IDAS, a solver for differential-algebraic systems with sensitivity analysis capabilities;
- KINSOL, a solver for nonlinear algebraic systems $F(u) = 0$.

3.2 IDAS organization

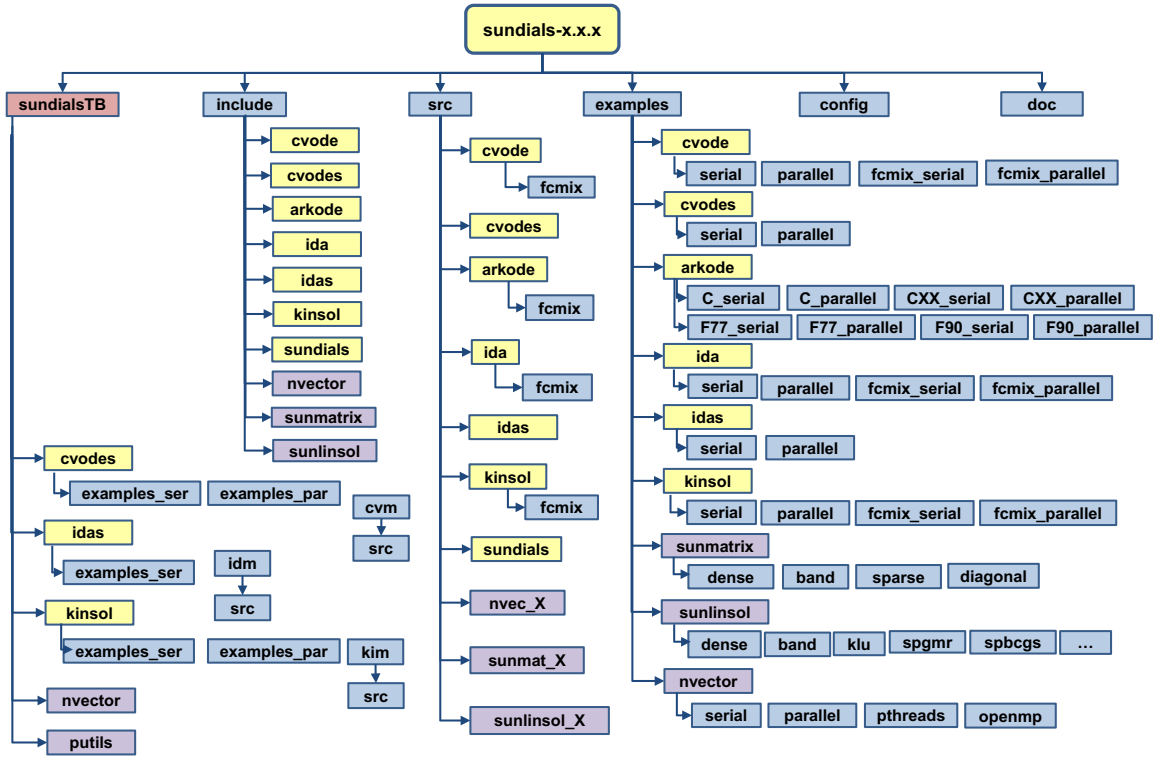
The IDAS package is written in the ANSI C language. The following summarizes the basic structure of the package, although knowledge of this structure is not necessary for its use.

The overall organization of the IDAS package is shown in Figure 3.2. The central integration module, implemented in the files `idas.h`, `idas_impl.h`, and `idas.c`, deals with the evaluation of integration coefficients, the Newton iteration process, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues. Although this module contains logic for the basic Newton iteration algorithm, it has no knowledge of the method being used to solve the linear systems that arise. For any given user problem, one of the linear system modules is specified, and is then invoked as needed during the integration.

In addition, if forward sensitivity analysis is turned on, the main module will integrate the forward sensitivity equations simultaneously with the original IVP. The sensitivity variables may be included in the local error control mechanism of the main integrator. IDAS provides two different strategies for dealing with the correction stage for the sensitivity variables: `IDA_SIMULTANEOUS` `IDA_STAGGERED` (see §2.5). The IDAS package includes an algorithm for the approximation of the sensitivity equations



(a) High-level diagram



(b) Directory structure of the source tree

Figure 3.1: Organization of the SUNDIALS suite

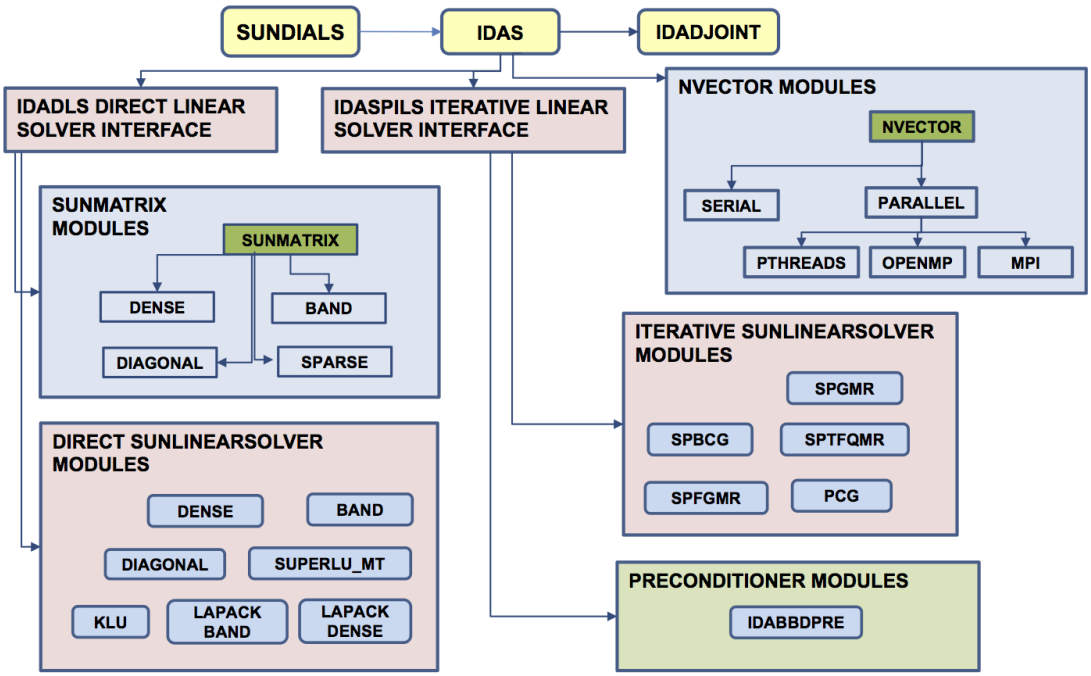


Figure 3.2: Overall structure diagram of the IDAS package. Modules specific to IDAS are distinguished by rounded boxes, while generic solver and auxiliary modules are in square boxes. Note that the direct linear solvers using Lapack implementations are not explicitly represented. Note also that the KLU and SuperLU_MT support is through interfaces to packages. Users will need to download and compile those packages independently.

residuals by difference quotients, but the user has the option of supplying these residual functions directly.

The adjoint sensitivity module (file `idaa.c`) provides the infrastructure needed for the backward integration of any system of DAEs which depends on the solution of the original IVP, in particular the adjoint system and any quadratures required in evaluating the gradient of the objective functional. This module deals with the setup of the checkpoints, the interpolation of the forward solution during the backward integration, and the backward integration of the adjoint equations.

At present, the package includes the following seven IDAS linear algebra modules, organized into two families. The *direct* family of linear solvers provides solvers for the direct solution of linear systems with dense or banded matrices and includes:

- IDADENSE: LU factorization and backsolving with dense matrices (using either an internal implementation or Blas/Lapack);
- IDABAND: LU factorization and backsolving with banded matrices (using either an internal implementation or Blas/Lapack);
- IDAKLU: LU factorization and backsolving with compressed-sparse-column (CSC) matrices using the KLU linear solver library [14, 1] (KLU to be downloaded and compiled by user independent of IDA);
- IDASUPERLUMT: LU factorization and backsolving with compressed-sparse-column (CSC) matrices using the threaded SuperLU_MT linear solver library [28, 15, 2] (SuperLU_MT to be downloaded and compiled by user independent of IDA).

The *spils* family of linear solvers provides scaled preconditioned iterative linear solvers and includes:

- IDASPGMR: scaled preconditioned GMRES method;
- IDASPBCG: scaled preconditioned Bi-CGStab method;
- IDASPTFQMR: scaled preconditioned TFQMR method.

The set of linear solver modules distributed with IDAS is intended to be expanded in the future as new algorithms are developed. Note that users wishing to employ KLU or SuperLU_MT will need to download and install these libraries independent of SUNDIALS. SUNDIALS provides only the interfaces between itself and these libraries.

In the case of the direct methods IDADENSE and IDABAND the package includes an algorithm for the approximation of the Jacobian by difference quotients, but the user also has the option of supplying the Jacobian (or an approximation to it) directly. When using the sparse direct linear solvers IDAKLU and IDASUPERLUMT the user must supply a routine for the Jacobian (or an approximation to it) in CSC format, since standard difference quotient approximations do not leverage the inherent sparsity of the problem. In the case of the Krylov iterative methods IDASPGMR, IDASPBCG, and IDASPTFQMR, the package includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector of appropriate length. Again, the user has the option of providing a routine for this operation. When using any of the Krylov methods, the user must supply the preconditioning in two phases: a setup phase (preprocessing of Jacobian data) and a solve phase. While there is no default choice of preconditioner analogous to the difference quotient approximation in the direct case, the references [4, 7], together with the example and demonstration programs included with IDAS, offer considerable assistance in building preconditioners.

Each IDAS linear solver module consists of five routines, devoted to (1) memory allocation and initialization, (2) setup of the matrix data involved, (3) solution of the system, (4) monitoring performance, and (5) freeing of memory. The setup and solution phases are separate because the evaluation of Jacobians and preconditioners is done only periodically during the integration, as required to achieve convergence. The call list within the central IDAS module to each of the five associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

These modules are also decomposed in another way. Each of the linear solver modules (IDADENSE etc.) consists of an interface built on top of a generic linear system solver (DENSE etc.). The interface deals with the use of the particular method in the IDAS context, whereas the generic solver is independent of the context. While some of the generic linear system solvers (DENSE, BAND, SPGMR, SPBCGS, and SPTFQMR) were written with SUNDIALS in mind, they are intended to be usable anywhere as general-purpose solvers. This separation also allows for any generic solver to be replaced by an improved version, with no necessity to revise the IDAS package elsewhere.

IDAS also provides a preconditioner module, IDABBDPRE, that works in conjunction with NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix.

All state information used by IDAS to solve a given problem is saved in a structure, and a pointer to that structure is returned to the user. There is no global data in the IDAS package, and so, in this respect, it is reentrant. State information specific to the linear solver is saved in a separate structure, a pointer to which resides in the IDAS memory structure. The reentrancy of IDAS was motivated by the situation where two or more problems are solved by intermixed calls to the package from one user program.

Chapter 4

Using IDAS for IVP Solution

This chapter is concerned with the use of IDAS for the integration of DAEs. The following sections treat the header files, the layout of the user's main program, description of the IDAS user-callable functions, and description of user-supplied functions. This usage is essentially equivalent to using IDA [24].

The sample programs described in the companion document [35] may also be helpful. Those codes may be used as templates (with the removal of some lines involved in testing), and are included in the IDAS package.

The user should be aware that not all linear solver modules are compatible with all NVECTOR implementations. For example, NVECTOR_PARALLEL is not compatible with the direct dense, direct band or direct sparse linear solvers, since these linear solver modules need to form the complete system Jacobian. The IDADENSE and IDABAND modules (using either the internal implementation or Lapack), as well as the IDAKLU and IDASUPERLUMT modules can only be used with NVECTOR_SERIAL, NVECTOR_OPENMP and NVECTOR_PTHREADS. It is not recommended to use a threaded vector module with SuperLU_MT unless it is the NVECTOR_OPENMP module and SuperLU_MT is also compiled with openMP. The preconditioner module IDABBDPRE can only be used with NVECTOR_PARALLEL.

IDAS uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in Appendix B.

4.1 Access to library and header files

At this point, it is assumed that the installation of IDAS, following the procedure described in Appendix A, has been completed successfully.

Regardless of where the user's application program resides, its associated compilation and load commands must make reference to the appropriate locations for the library and header files required by IDAS. The relevant library files are

- *libdir*`/libsundials_idas.`*lib*,
- *libdir*`/libsundials_nvec*.`*lib* (one to four files),

where the file extension *.lib* is typically `.so` for shared libraries and `.a` for static libraries. The relevant header files are located in the subdirectories

- *incdir*`/include/idas`
- *incdir*`/include/sundials`
- *incdir*`/include/nvector`

The directories *libdir* and *incdir* are the install library and include directories, respectively. For a default installation, these are *instdir*`/lib` and *instdir*`/include`, respectively, where *instdir* is the directory where SUNDIALS was installed (see Appendix A).

Note that an application cannot link to both the IDA and IDAS libraries because both contain user-callable functions with the same names (to ensure that IDAS is backward compatible with IDA). Therefore, applications that contain both DAE problems and DAEs with sensitivity analysis, should use IDAS.

4.2 Data types

The `sundials_types.h` file contains the definition of the type `realtype`, which is used by the SUNDIALS solvers for all floating-point data, the definition of the integer type `sunindextype`, which is used for vector and matrix indices, and `booleantype`, which is used for certain logic operations within SUNDIALS.

4.2.1 Floating point types

The type `realtype` can be `float`, `double`, or `long double`, with the default being `double`. The user can change the precision of the SUNDIALS solvers arithmetic at the configuration stage (see §A.1.2).

Additionally, based on the current precision, `sundials_types.h` defines `BIG_REAL` to be the largest value representable as a `realtype`, `SMALL_REAL` to be the smallest value representable as a `realtype`, and `UNIT_ROUNDOFF` to be the difference between 1.0 and the minimum `realtype` greater than 1.0.

Within SUNDIALS, real constants are set by way of a macro called `RCONST`. It is this macro that needs the ability to branch on the definition `realtype`. In ANSI C, a floating-point constant with no suffix is stored as a `double`. Placing the suffix "F" at the end of a floating point constant makes it a `float`, whereas using the suffix "L" makes it a `long double`. For example,

```
#define A 1.0
#define B 1.0F
#define C 1.0L
```

defines `A` to be a `double` constant equal to 1.0, `B` to be a `float` constant equal to 1.0, and `C` to be a `long double` constant equal to 1.0. The macro call `RCONST(1.0)` automatically expands to `1.0` if `realtype` is `double`, to `1.0F` if `realtype` is `float`, or to `1.0L` if `realtype` is `long double`. SUNDIALS uses the `RCONST` macro internally to declare all of its floating-point constants.

A user program which uses the type `realtype` and the `RCONST` macro to handle floating-point constants is precision-independent except for any calls to precision-specific standard math library functions. (Our example programs use both `realtype` and `RCONST`.) Users can, however, use the type `double`, `float`, or `long double` in their code (assuming that this usage is consistent with the typedef for `realtype`). Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use `realtype`, so long as the SUNDIALS libraries use the correct precision (for details see §A.1.2).

4.2.2 Integer types used for vector and matrix indices

The type `sunindextype` can be either a 64- or 32-bit *signed* integer. The default is the portable `int64_t` type, and the user can change it to `int32_t` at the configuration stage. The configuration system will detect if the compiler does not support portable types, and will replace `int64_t` and `int32_t` with `long long` and `int`, respectively, to ensure use of the desired sizes on Linux, Mac OS X and Windows platforms. SUNDIALS currently does not support *unsigned* integer types for vector and matrix indices, although these could be added in the future if there is sufficient demand.

A user program which uses `sunindextype` to handle vector and matrix indices will work with both index storage types except for any calls to index storage-specific external libraries. (Our `C` and `C++` example programs use `sunindextype`.) Users can, however, use any one of `int`, `long int`, `int32_t`, `int64_t` or `long long int` in their code, assuming that this usage is consistent with the typedef for `sunindextype` on their architecture). Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use `sunindextype`, so long as the SUNDIALS libraries use the appropriate index storage type (for details see §A.1.2).

4.3 Header files

The calling program must include several header files so that various macros and data types can be used. The header file that is always required is:

- `idas.h`, the header file for IDAS, which defines the several types and various constants, and includes function prototypes.

Note that `idas.h` includes `sundials_types.h`, which defines the types `realtype`, `sunindextype`, and `booleantype` and the constants `FALSE` and `TRUE`.

The calling program must also include an NVECTOR implementation header file, of the form `nvector_***.h`. See Chapter 7 for the appropriate name. This file in turn includes the header file `sundials_nvector.h` which defines the abstract `N_Vector` data type.

Finally, a linear solver module header file is required. The header files corresponding to the various linear solver options in IDAS are as follows:

- `idas_dense.h`, which is used with the dense direct linear solver;
- `idas_band.h`, which is used with the band direct linear solver;
- `idas_lapack.h`, which is used with Lapack implementations of dense or band direct linear solvers;
- `idas_klu.h`, which is used with the KLU sparse direct linear solver;
- `idas_superlumt.h`, which is used with the SuperLU_MT threaded sparse direct linear solver;
- `idas_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver SPGMR;
- `idas_spbcgs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver SPBCGS;
- `idas_sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov solver SPTFQMR.

The header files for the dense and banded linear solvers (both internal and Lapack) include the file `idas_direct.h`, which defines common functions. This in turn includes a file (`sundials_direct.h`) which defines the matrix type for these direct linear solvers (`DlsMat`), as well as various functions and macros acting on such matrices.

The header files for the KLU and SuperLU_MT sparse linear solvers include the file `idas_sparse.h`, which defines common functions. This in turn includes a file (`sundials_sparse.h`) which defines the matrix type for these sparse direct linear solvers (`SlsMat`), as well as various functions and macros acting on such matrices.

The header files for the Krylov iterative solvers include `idas_spils.h` which defines common functions and which in turn includes a header file (`sundials_iterative.h`) which enumerates the kind of preconditioning and (for the SPGMR solver only) the choices for the Gram-Schmidt process.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the `idasFoodWeb_kry_p` example (see [35]), preconditioning is done with a block-diagonal matrix. For this, even though the IDASPGMR linear solver is used, the header `sundials_dense.h` is included for access to the underlying generic dense linear solver.

4.4 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the integration of a DAE IVP. Most of the steps are independent of the NVECTOR implementation used. For the steps that are not, refer to Chapter 7 for the specific name of the function to be called or macro to be referenced.

1. **Initialize parallel or multi-threaded environment, if appropriate**

   For example, call `MPI_Init` to initialize MPI if used, or set `num_threads`, the number of threads to use within the threaded vector functions, if used.

2. **Set problem dimensions etc.**

   This generally includes the problem size `N`, and may include the local vector length `Nlocal`.

   Note: The variables `N` and `Nlocal` should be of type `sunindextype`.

3. **Set vectors of initial values**

   To set the vectors `y0` and `yp0` to initial values for y and $\dot{y}$, use the appropriate functions defined by the particular NVECTOR implementation.

   For native SUNDIALS vector implementations (except the CUDA and RAJA-based ones), use a call of the form `y0 = N_VMake_***(..., ydata)` if the `realtype` array `ydata` containing the initial values of y already exists. Otherwise, create a new vector by making a call of the form `y0 = N_VNew_***(...)`, and then set its elements by accessing the underlying data with a call of the form `ydata = N_VGetArrayPointer_***(y0)`. See §7.1-7.4 for details.

   For the *hypre* and PETSc vector wrappers, first create and initialize the underlying vector and then create NVECTOR wrapper with a call of the form `y0 = N_VMake_***(yvec)`, where `yvec` is a *hypre* or PETSc vector. Note that calls like `N_VNew_***(...)` and `N_VGetArrayPointer_***(...)` are not available for these vector wrappers. See §7.5 and §7.6 for details.

   If using either the CUDA- or RAJA-based vector implementations use a call of the form `y0 = N_VMake_***(..., c)` where `c` is a pointer to a `suncudavec` or `sunrajavec` vector class if this class already exists. Otherwise, create a new vector by making a call of the form `y0 = N_VNew_***(...)`, and then set its elements by accessing the underlying data where it is located with a call of the form `N_VGetDeviceArrayPointer_***` or `N_VGetHostArrayPointer_***`. Note that the vector class will allocate memory on both the host and device when instantiated. See §7.7-7.8 for details.

   Set the vector `yp0` of initial conditions for $\dot{y}$ similarly.

4. **Create IDAS object**

   Call `ida_mem = IDACreate()` to create the IDAS memory block. `IDACreate` returns a pointer to the IDAS memory structure. See §4.5.1 for details. This `void *` pointer must then be passed as the first argument to all subsequent IDAS function calls.

5. **Initialize IDAS solver**

   Call `IDAInit(...)` to provide required problem specifications (residual function, initial time, and initial conditions), allocate internal memory for IDAS, and initialize IDAS. `IDAInit` returns an error flag to indicate success or an illegal argument value. See §4.5.1 for details.

6. **Specify integration tolerances**

   Call `IDASStolerances(...)` or `IDASVtolerances(...)` to specify, respectively, a scalar relative tolerance and scalar absolute tolerance, or a scalar relative tolerance and a vector of absolute tolerances. Alternatively, call `IDAWFtolerances` to specify a function which sets directly the weights used in evaluating WRMS vector norms. See §4.5.2 for details.

7. **Set optional inputs**

   Optionally, call `IDASet*` functions to change from their default values any optional inputs that control the behavior of IDAS. See §4.5.7.1 for details.

8. **Attach linear solver module**

   Initialize the linear solver module with one of the following calls (for details see §4.5.3):

```
flag = IDADense(...);
flag = IDABand(...);
flag = IDALapackDense(...);
flag = IDALapackBand(...);
flag = IDAKLU(...);
flag = IDASuperLUMT(...);
flag = IDASpgmr(...);
flag = IDASpbcg(...);
flag = IDASptfqmr(...);
```

NOTE: The direct (dense or band) and sparse linear solver options are usable only in a serial environment.

9. **Set linear solver optional inputs**

   Optionally, call `IDA*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See §4.5.7.2 and §4.5.7.4 for details.

10. **Correct initial values**

    Optionally, call `IDACalcIC` to correct the initial values `y0` and `yp0` passed to `IDAInit`. See §4.5.4. Also see §4.5.7.5 for relevant optional input calls.

11. **Specify rootfinding problem**

    Optionally, call `IDARootInit` to initialize a rootfinding problem to be solved during the integration of the DAE system. See §4.5.5 for details, and see §4.5.7.6 for relevant optional input calls.

12. **Advance solution in time**

    For each point at which output is desired, call `flag = IDASolve(ida_mem, tout, &tret, yret, ypret, itask)`. Here `itask` specifies the return mode. The vector `yret` (which can be the same as the vector `y0` above) will contain $y(t)$, while the vector `ypret` will contain $\dot{y}(t)$. See §4.5.6 for details.

13. **Get optional outputs**

    Call `IDA*Get*` functions to obtain optional output. See §4.5.9 for details.

14. **Deallocate memory for solution vectors**

    Upon completion of the integration, deallocate memory for the vectors `yret` and `ypret` (or `y` and `yp`) by calling the appropriate destructor function defined by the NVECTOR implementation:

    ```
    N_VDestroy_***(yret);
    ```

    and similarly for `ypret`.

15. **Free solver memory**

    `IDAFree(&ida_mem)` to free the memory allocated for IDAS.

16. **Finalize MPI, if used**

    Call `MPI_Finalize()` to terminate MPI.

SUNDIALS provides some linear solvers only as a means for users to get problems running and not as highly efficient solvers. For example, if solving a dense system, we suggest using the Lapack solvers if the size of the linear system is $> 50,000$. (Thanks to A. Nicolai for his testing and recommendation.)

Table 4.1 shows the linear solver interfaces available as SUNLINSOL modules and the vector implementations required for use. As an example, one cannot use the dense direct solver interfaces with the MPI-based vector implementation. However, as discussed in Chapter 9 the SUNDIALS packages operate on generic SUNLINSOL objects, allowing a user to develop their own solvers should they so desire.

Table 4.1: SUNDIALS linear solver interfaces and vector implementations that can be used for each.

Linear Solver	Serial	Parallel (MPI)	OpenMP	pThreads	*hypre*	PETSc	CUDA	RAJA	User Supp.
Dense	✓		✓	✓					✓
Band	✓		✓	✓					✓
LapackDense	✓		✓	✓					✓
LapackBand	✓		✓	✓					✓
KLU	✓		✓	✓					✓
SUPERLUMT	✓		✓	✓					✓
SPGMR	✓	✓	✓	✓	✓	✓	✓	✓	✓
SPFGMR	✓	✓	✓	✓	✓	✓	✓	✓	✓
SPBCGS	✓	✓	✓	✓	✓	✓	✓	✓	✓
SPTFQMR	✓	✓	✓	✓	✓	✓	✓	✓	✓
PCG	✓	✓	✓	✓	✓	✓	✓	✓	✓
User Supp.	✓	✓	✓	✓	✓	✓	✓	✓	✓

4.5 User-callable functions

This section describes the IDAS functions that are called by the user to set up and solve a DAE. Some of these are required. However, starting with §4.5.7, the functions listed involve optional inputs/outputs or restarting, and those paragraphs can be skipped for a casual use of IDAS. In any case, refer to §4.4 for the correct order of these calls.

On an error, each user-callable function returns a negative value and sends an error message to the error handler routine, which prints the message on `stderr` by default. However, the user can set a file as error output or can provide his own error handler function (see §4.5.7.1).

4.5.1 IDAS initialization and deallocation functions

The following three functions must be called in the order listed. The last one is to be called only after the DAE solution is complete, as it frees the IDAS memory block created and allocated by the first two calls.

`IDACreate`

Call `ida_mem = IDACreate();`

Description The function `IDACreate` instantiates an IDAS solver object.

Arguments `IDACreate` has no arguments.

Return value If successful, `IDACreate` returns a pointer to the newly created IDAS memory block (of type `void *`). Otherwise it returns `NULL`.

`IDAInit`

Call `flag = IDAInit(ida_mem, res, t0, y0, yp0);`

Description The function `IDAInit` provides required problem and solution specifications, allocates internal memory, and initializes IDAS.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

`res` (`IDAResFn`) is the C function which computes the residual function F in the DAE. This function has the form `res(t, yy, yp, resval, user_data)`. For full details see §4.6.1.

`t0` (`realtype`) is the initial value of t.

`y0` (`N_Vector`) is the initial value of y.

`yp0` (`N_Vector`) is the initial value of $\dot{y}$.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS` The call to `IDAInit` was successful.

`IDA_MEM_NULL` The IDAS memory block was not initialized through a previous call to `IDACreate`.

`IDA_MEM_FAIL` A memory allocation request has failed.

`IDA_ILL_INPUT` An input argument to `IDAInit` has an illegal value.

Notes If an error occurred, `IDAInit` also sends an error message to the error handler function.

`IDAFree`

Call `IDAFree(&ida_mem);`

Description The function `IDAFree` frees the pointer allocated by a previous call to `IDACreate`.

Arguments The argument is the pointer to the IDAS memory block (of type `void *`).

Return value The function `IDAFree` has no return value.

4.5.2 IDAS tolerance specification functions

One of the following three functions must be called to specify the integration tolerances (or directly specify the weights used in evaluating WRMS vector norms). Note that this call must be made after the call to `IDAInit`.

`IDASStolerances`

Call `flag = IDASStolerances(ida_mem, reltol, abstol);`

Description The function `IDASStolerances` specifies scalar relative and absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

`reltol` (`realtype`) is the scalar relative error tolerance.

`abstol` (`realtype`) is the scalar absolute error tolerance.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS` The call to `IDASStolerances` was successful.

`IDA_MEM_NULL` The IDAS memory block was not initialized through a previous call to `IDACreate`.

`IDA_NO_MALLOC` The allocation function `IDAInit` has not been called.

`IDA_ILL_INPUT` One of the input tolerances was negative.

`IDASVtolerances`

Call `flag = IDASVtolerances(ida_mem, reltol, abstol);`

Description The function `IDASVtolerances` specifies scalar relative tolerance and vector absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
`reltol` (`realtype`) is the scalar relative error tolerance.
`abstol` (`N_Vector`) is the vector of absolute error tolerances.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASVtolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_MALLOC`	The allocation function `IDAInit` has not been called.
`IDA_ILL_INPUT`	The relative error tolerance was negative or the absolute tolerance had a negative component.

Notes This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the state vector y.

`IDAWFtolerances`

Call `flag = IDAWFtolerances(ida_mem, efun);`

Description The function `IDAWFtolerances` specifies a user-supplied function `efun` that sets the multiplicative error weights W_i for use in the weighted RMS norm, which are normally defined by Eq. (2.7).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
`efun` (`IDAEwtFn`) is the C function which defines the `ewt` vector (see §4.6.3).

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDAWFtolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_MALLOC`	The allocation function `IDAInit` has not been called.

General advice on choice of tolerances. For many users, the appropriate choices for tolerance values in `reltol` and `abstol` are a concern. The following pieces of advice are relevant.

(1) The scalar relative tolerance `reltol` is to be set to control relative errors. So `reltol`=10^{-4} means that errors are controlled to .01%. We do not recommend using `reltol` larger than 10^{-3}. On the other hand, `reltol` should not be so small that it is comparable to the unit roundoff of the machine arithmetic (generally around 10^{-15}).

(2) The absolute tolerances `abstol` (whether scalar or vector) need to be set to control absolute errors when any components of the solution vector `y` may be so small that pure relative error control is meaningless. For example, if `y[i]` starts at some nonzero value, but in time decays to zero, then pure relative error control on `y[i]` makes no sense (and is overly costly) after `y[i]` is below some noise level. Then `abstol` (if scalar) or `abstol[i]` (if a vector) needs to be set to that noise level. If the different components have different noise levels, then `abstol` should be a vector. See the example `idasRoberts_dns` in the IDAS package, and the discussion of it in the IDAS Examples document [35]. In that problem, the three components vary between 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

(3) Finally, it is important to pick all the tolerance values conservatively, because they control the error committed on each individual time step. The final (global) errors are a sort of accumulation of those per-step errors. A good rule of thumb is to reduce the tolerances by a factor of .01 from the actual

desired limits on errors. So if you want .01% accuracy (globally), a good choice is `reltol`$= 10^{-6}$. But in any case, it is a good idea to do a few experiments with the tolerances to see how the computed solution values vary as tolerances are reduced.

Advice on controlling unphysical negative values. In many applications, some components in the true solution are always positive or non-negative, though at times very small. In the numerical solution, however, small negative (hence unphysical) values can then occur. In most cases, these values are harmless, and simply need to be controlled, not eliminated. The following pieces of advice are relevant.

(1) The way to control the size of unwanted negative computed values is with tighter absolute tolerances. Again this requires some knowledge of the noise level of these components, which may or may not be different for different components. Some experimentation may be needed.

(2) If output plots or tables are being generated, and it is important to avoid having negative numbers appear there (for the sake of avoiding a long explanation of them, if nothing else), then eliminate them, but only in the context of the output medium. Then the internal values carried by the solver are unaffected. Remember that a small negative value in `yret` returned by IDAS, with magnitude comparable to `abstol` or less, is equivalent to zero as far as the computation is concerned.

(3) The user's residual routine `res` should never change a negative value in the solution vector `yy` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `res` routine cannot tolerate a zero or negative value (e.g. because there is a square root or log of it), then the offending value should be changed to zero or a tiny positive number in a temporary variable (not in the input `yy` vector) for the purposes of computing $F(t, y, \dot{y})$.

(4) IDAS provides the option of enforcing positivity or non-negativity on components. Also, such constraints can be enforced by use of the recoverable error return feature in the user-supplied residual function. However, because these options involve some extra overhead cost, they should only be exercised if the use of absolute tolerances to control the computed values is unsuccessful.

4.5.3 Linear solver specification functions

As previously explained, Newton iteration requires the solution of linear systems of the form (2.5). There are seven IDAS linear solvers currently available for this task: IDADENSE, IDABAND, IDAKLU, IDASUPERLUMT, IDASPGMR, IDASPBCG, and IDASPTFQMR.

The first two linear solvers are direct and derive their names from the type of approximation used for the Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial \dot{y}$. IDADENSE and IDABAND work with dense and banded approximations to J, respectively. The SUNDIALS suite includes both internal implementations of these two linear solvers and interfaces to Lapack implementations. Together, these linear solvers are referred to as IDADLS (from Direct Linear Solvers).

The second two linear solvers are sparse direct solvers based on Gaussian elimination, and require user-supplied routines to construct the Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial \dot{y}$ in compressed-sparse-column format. The SUNDIALS suite does not include internal implementations of these solver libraries, instead requiring compilation of SUNDIALS to link with existing installations of these libraries (if either is missing, SUNDIALS will install without the corresponding interface routines). Together, these linear solvers are referred to as CVSLS (from Sparse Linear Solvers).

The remaining three IDAS linear solvers, IDASPGMR, IDASPBCG, and IDASPTFQMR, are Krylov iterative solvers. The SPGMR, SPBCGS, and SPTFQMR in the names indicate the scaled preconditioned GMRES, scaled preconditioned Bi-CGStab, and scaled preconditioned TFQMR methods, respectively. Together, they are referred to as IDASPILS (from Scaled Preconditioned Iterative Linear Solvers).

When using any of the Krylov linear solvers, preconditioning (on the left) is permitted, and in fact encouraged, for the sake of efficiency. A preconditioner matrix P must approximate the Jacobian J, at least crudely. For the specification of a preconditioner, see §4.5.7.4 and §4.6.

To specify an IDAS linear solver, after the call to `IDACreate` but before any calls to `IDASolve`, the user's program must call one of the functions `IDADense`/`IDALapackDense`, `IDABand`/`IDALapackBand`, `IDAKLU`, `IDASuperLUMT`, `IDASpgmr`, `IDASpbcg`, or `IDASptfqmr`, as documented below. The first argument passed to these functions is the IDAS memory pointer returned by `IDACreate`. A call to one

of these functions links the main IDAS integrator to a linear solver and allows the user to specify parameters which are specific to a particular solver, such as the bandwidths in the IDABAND case. The use of each of the linear solvers involves certain constants and possibly some macros, that are likely to be needed in the user code. These are available in the corresponding header file associated with the linear solver, as specified below.

In each case the linear solver module used by IDAS is actually built on top of a generic linear system solver, which may be of interest in itself. These generic solvers, denoted DENSE, BAND, KLU, SUPERLUMT, SPGMR, SPBCGS, and SPTFQMR, are described separately in Chapter 11.

`IDADense`

Call `flag = IDADense(ida_mem, N);`

Description The function `IDADense` selects the IDADENSE linear solver and indicates the use of the internal direct dense linear algebra functions.

The user's main program must include the `idas_dense.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`N` (`sunindextype`) problem dimension.

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS`	The IDADENSE initialization was successful.
`IDADLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADLS_ILL_INPUT`	The IDADENSE solver is not compatible with the current NVECTOR module.
`IDADLS_MEM_FAIL`	A memory allocation request failed.

Notes The IDADENSE linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS are compatible.

`IDALapackDense`

Call `flag = IDALapackDense(ida_mem, N);`

Description The function `IDALapackDense` selects the IDADENSE linear solver and indicates the use of Lapack functions.

The user's main program must include the `idas_lapack.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`N` (`int`) problem dimension.

Return value The values of the returned `flag` (of type `int`) are identical to those of `IDADense`.

Notes Note that `N` is restricted to be of type `int` here, because of the corresponding type restriction in the Lapack solvers.

`IDABand`

Call `flag = IDABand(ida_mem, N, mupper, mlower);`

Description The function `IDABand` selects the IDABAND linear solver and indicates the use of the internal direct band linear algebra functions.

The user's main program must include the `idas_band.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`N` (`sunindextype`) problem dimension.
`mupper` (`sunindextype`) upper half-bandwidth of the problem Jacobian (or of the approximation of it).

`mlower` (`sunindextype`) lower half-bandwidth of the problem Jacobian (or of the approximation of it).

Return value The return value `flag` (of type `int`) is one of

`IDABAND_SUCCESS` The IDABAND initialization was successful.

`IDABAND_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDABAND_ILL_INPUT` The IDABAND solver is not compatible with the current NVECTOR module, or one of the Jacobian half-bandwidths is outside its valid range ($0 \ldots$ `N`-1).

`IDABAND_MEM_FAIL` A memory allocation request failed.

Notes The IDABAND linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only NVECTOR_SERIAL, NVECTOR_OPENMP and NVECTOR_PTHREADS are compatible. The half-bandwidths are to be set so that the nonzero locations (i, j) in the banded (approximate) Jacobian satisfy $-$`mlower` $\leq j - i \leq$ `mupper`.

`IDALapackBand`

Call `flag = IDALapackBand(ida_mem, N, mupper, mlower);`

Description The function `IDALapackBand` selects the IDABAND linear solver and indicates the use of Lapack functions.

The user's main program must include the `idas_lapack.h` header file.

Arguments The input arguments are identical to those of `IDABand`, except that `N`, `mupper`, and `mlower` are of type `int` here.

Return value The values of the returned `flag` (of type `int`) are identical to those of `IDABand`.

Notes Note that `N`, `mupper`, and `mlower` are restricted to be of type `int` here, because of the corresponding type restriction in the Lapack solvers.

`IDAKLU`

Call `flag = IDAKLU(ida_mem, NP, NNZ, sparsetype);`

Description The function `IDAKLU` selects the IDAKLU linear solver and indicates the use of sparse direct linear algebra functions.

The user's main program must include the `idas_sparse.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`NP` (`int`) problem dimension.

`NNZ` (`int`) maximum number of nonzero entries in the system Jacobian.

`sparsetype` (`int`) sparse storage type of the system Jacobian. If `sparsetype` is set to `CSC_MAT` the solver will expect the Jacobian to be stored as a compressed sparse column matrix, and if `sparsetype=CSR_MAT` the solver will expect a compressed sparse row matrix. If neither option is chosen, the solver will exit with error.

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS` The IDAKLU initialization was successful.

`IDASLS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASLS_ILL_INPUT` The IDAKLU solver is not compatible with the current NVECTOR module.

`IDASLS_MEM_FAIL` A memory allocation request failed.

`IDASLS_PACKAGE_FAIL` A call to the KLU library returned a failure flag.

Notes The IDAKLU linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only NVECTOR_SERIAL, NVECTOR_OPENMP and NVECTOR_PTHREADS are compatible.

`IDASuperLUMT`

Call `flag = IDASuperLUMT(ida_mem, num_threads, N, NNZ);`

Description The function `IDASuperLUMT` selects the IDASUPERLUMT linear solver and indicates the use of sparse direct linear algebra functions.

The user's main program must include the `idas_superlumt.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`num_threads` (`int`) the number of threads to use when factoring/solving the linear systems. Note that SuperLU_MT is thread-parallel only in the factorization routine.

`N` (`int`) problem dimension.

`NNZ` (`int`) maximum number of nonzero entries in the system Jacobian.

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS` The IDASUPERLUMT initialization was successful.

`IDASLS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASLS_ILL_INPUT` The IDASUPERLUMT solver is not compatible with the current NVECTOR module.

`IDASLS_MEM_FAIL` A memory allocation request failed.

`IDASLS_PACKAGE_FAIL` A call to the SuperLU_MT library returned a failure flag.

Notes The IDASUPERLUMT linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only NVECTOR_SERIAL, NVECTOR_OPENMP and NVECTOR_PTHREADS are compatible.

Performance will significantly degrade if the user applies the SuperLU_MT package compiled with PThreads while using the NVECTOR_OPENMP module. If a user wants to use a threaded vector kernel with this thread-parallel solver, then SuperLU_MT should be compiled with openMP and the NVECTOR_OPENMP module should be used. Also, note that the expected benefit of using the threaded vector kernel is minimal compared to the potential benefit of the threaded solver, unless very long (greater than 100,000 entries) vectors are used.

`IDASpgmr`

Call `flag = IDASpgmr(ida_mem, maxl);`

Description The function `IDASpgmr` selects the IDASPGMR linear solver.

The user's main program must include the `idas_spgmr.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPILS_MAXL`= 5.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPGMR initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

IDASpbcg

Call `flag = IDASpbcg(ida_mem, maxl);`

Description The function `IDASpbcg` selects the IDASPBCG linear solver.

The user's main program must include the `idas_spbcgs.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPILS_MAXL`= 5.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPBCG initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

IDASptfqmr

Call `flag = IDASptfqmr(ida_mem, maxl);`

Description The function `IDASptfqmr` selects the IDASPTFQMR linear solver.

The user's main program must include the `idas_sptfqmr.h` header file.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `IDA_SPILS_MAXL`= 5.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The IDASPTFQMR initialization was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_MEM_FAIL` A memory allocation request failed.

4.5.4 Initial condition calculation function

`IDACalcIC` calculates corrected initial conditions for the DAE system for certain index-one problems including a class of systems of semi-implicit form. (See §2.1 and Ref. [6].) It uses Newton iteration combined with a linesearch algorithm. Calling `IDACalcIC` is optional. It is only necessary when the initial conditions do not satisfy the given system. Thus if `y0` and `yp0` are known to satisfy $F(t_0, y_0, \dot{y}_0) = 0$, then a call to `IDACalcIC` is generally *not* necessary.

A call to the function `IDACalcIC` must be preceded by successful calls to `IDACreate` and `IDAInit` (or `IDAReInit`), and by a successful call to the linear system solver specification function. The call to `IDACalcIC` should precede the call(s) to `IDASolve` for the given problem.

IDACalcIC

Call `flag = IDACalcIC(ida_mem, icopt, tout1);`

Description The function `IDACalcIC` corrects the initial values `y0` and `yp0` at time `t0`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`icopt` (`int`) is one of the following two options for the initial condition calculation.

`icopt`=`IDA_YA_YDP_INIT` directs `IDACalcIC` to compute the algebraic components of y and differential components of $\dot{y}$, given the differential components of y. This option requires that the `N_Vector id` was set through `IDASetId`, specifying the differential and algebraic components.

`icopt`=`IDA_Y_INIT` directs `IDACalcIC` to compute all components of y, given $\dot{y}$. In this case, `id` is not required.

`tout1` (`realtype`) is the first value of t at which a solution will be requested (from `IDASolve`). This value is needed here only to determine the direction of integration and rough scale in the independent variable t.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	`IDASolve` succeeded.
`IDA_MEM_NULL`	The argument `ida_mem` was `NULL`.
`IDA_NO_MALLOC`	The allocation function `IDAInit` has not been called.
`IDA_ILL_INPUT`	One of the input arguments was illegal.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_LINIT_FAIL`	The linear solver's initialization function failed.
`IDA_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`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_FIRST_RES_FAIL`	The user's residual function returned a recoverable error flag on the first call, but `IDACalcIC` was unable to recover.
`IDA_RES_FAIL`	The user's residual function returned a nonrecoverable error flag.
`IDA_NO_RECOVERY`	The user's residual function, or the linear solver's setup or solve function 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, and within the allowed number of backtracks.
`IDA_CONV_FAIL`	`IDACalcIC` failed to get convergence of the Newton iterations.

Notes All failure return values are negative and therefore a test `flag` < 0 will trap all `IDACalcIC` failures.

Note that `IDACalcIC` will correct the values of $y(t_0)$ and $\dot{y}(t_0)$ which were specified in the previous call to `IDAInit` or `IDAReInit`. To obtain the corrected values, call `IDAGetconsistentIC` (see §4.5.9.3).

4.5.5 Rootfinding initialization function

While integrating the IVP, IDAS has the capability of finding the roots of a set of user-defined functions. To activate the rootfinding algorithm, call the following function. This is normally called only once, prior to the first call to `IDASolve`, but if the rootfinding problem is to be changed during the solution, `IDARootInit` can also be called prior to a continuation call to `IDASolve`.

`IDARootInit`

Call `flag = IDARootInit(ida_mem, nrtfn, g);`

Description The function `IDARootInit` specifies that the roots of a set of functions $g_i(t, y, \dot{y})$ are to be found while the IVP is being solved.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

`nrtfn` (`int`) is the number of root functions g_i.

`g` (`IDARootFn`) is the C function which defines the `nrtfn` functions $g_i(t, y, \dot{y})$ whose roots are sought. See §4.6.4 for details.

Return value The return value `flag` (of type `int`) is one of

IDA_SUCCESS	The call to IDARootInit was successful.
IDA_MEM_NULL	The ida_mem argument was NULL.
IDA_MEM_FAIL	A memory allocation failed.
IDA_ILL_INPUT	The function g is NULL, but nrtfn> 0.

Notes If a new IVP is to be solved with a call to IDAReInit, where the new IVP has no rootfinding problem but the prior one did, then call IDARootInit with nrtfn= 0.

4.5.6 IDAS solver function

This is the central step in the solution process, the call to perform the integration of the DAE. One of the input arguments (itask) specifies one of two modes as to where IDAS is to return a solution. But these modes are modified if the user has set a stop time (with IDASetStopTime) or requested rootfinding.

IDASolve

Call `flag = IDASolve(ida_mem, tout, &tret, yret, ypret, itask);`

Description The function IDASolve integrates the DAE over an interval in t.

Arguments

ida_mem	(void *) pointer to the IDAS memory block.
tout	(realtype) the next time at which a computed solution is desired.
tret	(realtype) the time reached by the solver (output).
yret	(N_Vector) the computed solution vector y.
ypret	(N_Vector) the computed solution vector $\dot{y}$.
itask	(int) a flag indicating the job of the solver for the next user step. The IDA_NORMAL task is to have the solver take internal steps until it has reached or just passed the user specified tout parameter. The solver then interpolates in order to return approximate values of y(tout) and $\dot{y}$(tout). The IDA_ONE_STEP option tells the solver to just take one internal step and return the solution at the point reached by that step.

Return value IDASolve returns vectors yret and ypret and a corresponding independent variable value t = tret, such that (yret, ypret) are the computed values of ($y(t)$, $\dot{y}(t)$).

In IDA_NORMAL mode with no errors, tret will be equal to tout and yret = y(tout), ypret = $\dot{y}$(tout).

The return value flag (of type int) will be one of the following:

IDA_SUCCESS	IDASolve succeeded.
IDA_TSTOP_RETURN	IDASolve succeeded by reaching the stop point specified through the optional input function IDASetStopTime.
IDA_ROOT_RETURN	IDASolve succeeded and found one or more roots. In this case, tret is the location of the root. If nrtfn > 1, call IDAGetRootInfo to see which g_i were found to have a root. See §4.5.9.4 for more information.
IDA_MEM_NULL	The ida_mem argument was NULL.
IDA_ILL_INPUT	One of the inputs to IDASolve was illegal, or some other input to the solver was either illegal or missing. The latter category includes the following situations: (a) The tolerances have not been set. (b) A component of the error weight vector became zero during internal time-stepping. (c) The linear solver initialization function (called by the user after calling IDACreate) failed to set the linear solver-specific lsolve field in ida_mem. (d) A root of one of the root functions was found both at a point t and also very near t. In any case, the user should see the printed error message for details.

`IDA_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tout`. The default value for `mxstep` is `MXSTEP_DEFAULT = 500`.
`IDA_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`IDA_ERR_FAIL`	Error test failures occurred too many times (`MXNEF = 10`) during one internal time step or occurred with $\|h\| = h_{min}$.
`IDA_CONV_FAIL`	Convergence test failures occurred too many times (`MXNCF = 10`) during one internal time step or occurred with $\|h\| = h_{min}$.
`IDA_LINIT_FAIL`	The linear solver's initialization function failed.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`IDA_CONSTR_FAIL`	The inequality constraints were violated and the solver was unable to recover.
`IDA_REP_RES_ERR`	The user's residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
`IDA_RES_FAIL`	The user's residual function returned a nonrecoverable error flag.
`IDA_RTFUNC_FAIL`	The rootfinding function failed.

Notes The vector `yret` can occupy the same space as the vector `y0` of initial conditions that was passed to `IDAInit`, and the vector `ypret` can occupy the same space as `yp0`.

In the `IDA_ONE_STEP` mode, `tout` is used on the first call only, and only to get the direction and rough scale of the independent variable.

All failure return values are negative and therefore a test `flag` < 0 will trap all `IDASolve` failures.

On any error return in which one or more internal steps were taken by `IDASolve`, the returned values of `tret`, `yret`, and `ypret` correspond to the farthest point reached in the integration. On all other error returns, these values are left unchanged from the previous `IDASolve` return.

4.5.7 Optional input functions

There are numerous optional input parameters that control the behavior of the IDAS solver. IDAS provides functions that can be used to change these optional input parameters from their default values. Table 4.2 lists all optional input functions in IDAS which are then described in detail in the remainder of this section. For the most casual use of IDAS, the reader can skip to §4.6.

We note that, on an error return, all these functions also send an error message to the error handler function. We also note that all error return values are negative, so a test `flag` < 0 will catch any error.

4.5.7.1 Main solver optional input functions

The calls listed here can be executed in any order. However, if the user's program calls either `IDASetErrFile` or `IDASetErrHandlerFn`, then that call should appear first, in order to take effect for any later error message.

`IDASetErrFile`

Call `flag = IDASetErrFile(ida_mem, errfp);`

Description The function `IDASetErrFile` specifies the pointer to the file where all IDAS messages should be directed when the default IDAS error handler function is used.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

Table 4.2: Optional inputs for IDAS, IDADLS, IDASLS, and IDASPILS

Optional input	Function name	Default
IDAS main solver		
Pointer to an error file	`IDASetErrFile`	`stderr`
Error handler function	`IDASetErrHandlerFn`	internal fn.
User data	`IDASetUserData`	`NULL`
Maximum order for BDF method	`IDASetMaxOrd`	5
Maximum no. of internal steps before t_{out}	`IDASetMaxNumSteps`	500
Initial step size	`IDASetInitStep`	estimated
Maximum absolute step size	`IDASetMaxStep`	∞
Value of t_{stop}	`IDASetStopTime`	∞
Maximum no. of error test failures	`IDASetMaxErrTestFails`	10
Maximum no. of nonlinear iterations	`IDASetMaxNonlinIters`	4
Maximum no. of convergence failures	`IDASetMaxConvFails`	10
Maximum no. of error test failures	`IDASetMaxErrTestFails`	7
Coeff. in the nonlinear convergence test	`IDASetNonlinConvCoef`	0.33
Suppress alg. vars. from error test	`IDASetSuppressAlg`	`FALSE`
Variable types (differential/algebraic)	`IDASetId`	`NULL`
Inequality constraints on solution	`IDASetConstraints`	`NULL`
Direction of zero-crossing	`IDASetRootDirection`	both
Disable rootfinding warnings	`IDASetNoInactiveRootWarn`	none
IDAS initial conditions calculation		
Coeff. in the nonlinear convergence test	`IDASetNonlinConvCoefIC`	0.0033
Maximum no. of steps	`IDASetMaxNumStepsIC`	5
Maximum no. of Jacobian/precond. evals.	`IDASetMaxNumJacsIC`	4
Maximum no. of Newton iterations	`IDASetMaxNumItersIC`	10
Max. linesearch backtracks per Newton iter.	`IDASetMaxBacksIC`	100
Turn off linesearch	`IDASetLineSearchOffIC`	`FALSE`
Lower bound on Newton step	`IDASetStepToleranceIC`	$\text{uround}^{2/3}$
IDADLS linear solvers		
Dense Jacobian function	`IDADlsSetDenseJacFn`	DQ
Band Jacobian function	`IDADlsSetBandJacFn`	DQ
IDASLS linear solvers		
Sparse Jacobian function	`IDASlsSetSparseJacFn`	none
Sparse matrix ordering algorithm	`IDAKLUSetOrdering`	1 for `COLAMD`
Sparse matrix ordering algorithm	`IDASuperLUMTSetOrdering`	3 for `COLAMD`
IDASPILS linear solvers		
Preconditioner functions	`IDASpilsSetPreconditioner`	NULL, NULL
Jacobian-times-vector function	`IDASpilsSetJacTimesVecFn`	DQ
Factor in linear convergence test	`IDASpilsSetEpsLin`	0.05
Factor in DQ increment calculation	`IDASpilsSetIncrementFactor`	1.0
Maximum no. of restarts (IDASPGMR)	`IDASpilsSetMaxRestarts`	5
Type of Gram-Schmidt orthogonalization [(a)]	`IDASpilsSetGSType`	Modified GS
Maximum Krylov subspace size[(b)]	`IDASpilsSetMaxl`	5

[(a)] Only for IDASPGMR

[(b)] Only for IDASPBCG and IDASPTFQMR

`errfp` (`FILE *`) pointer to output file.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value for `errfp` is `stderr`.

Passing a value `NULL` disables all future error message output (except for the case in which the IDAS memory pointer is `NULL`). This use of `IDASetErrFile` is strongly discouraged.

If `IDASetErrFile` is to be called, it should be called before any other optional input functions, in order to take effect for any later error message.

`IDASetErrHandlerFn`

Call `flag = IDASetErrHandlerFn(ida_mem, ehfun, eh_data);`

Description The function `IDASetErrHandlerFn` specifies the optional user-defined function to be used in handling error messages.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`ehfun` (`IDAErrHandlerFn`) is the user's C error handler function (see §4.6.2).

`eh_data` (`void *`) pointer to user data passed to `ehfun` every time it is called.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The function `ehfun` and data pointer `eh_data` have been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes Error messages indicating that the IDAS solver memory is `NULL` will always be directed to `stderr`.

`IDASetUserData`

Call `flag = IDASetUserData(ida_mem, user_data);`

Description The function `IDASetUserData` specifies the user data block `user_data` and attaches it to the main IDAS memory block.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`user_data` (`void *`) pointer to the user data.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes If specified, the pointer to `user_data` is passed to all user-supplied functions that have it as an argument. Otherwise, a `NULL` pointer is passed.

If `user_data` is needed in user linear solver or preconditioner functions, the call to `IDASetUserData` must be made *before* the call to specify the linear solver.

`IDASetMaxOrd`

Call `flag = IDASetMaxOrd(ida_mem, maxord);`

Description The function `IDASetMaxOrd` specifies the maximum order of the linear multistep method.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxord` (`int`) value of the maximum method order. This must be positive.

Return value The return value `flag` (of type `int`) is one of

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

IDA_ILL_INPUT The input value maxord is ≤ 0, or larger than its previous value.

Notes The default value is 5. If the input value exceeds 5, the value 5 will be used. Since maxord affects the memory requirements for the internal IDAS memory block, its value cannot be increased past its previous value.

IDASetMaxNumSteps

Call `flag = IDASetMaxNumSteps(ida_mem, mxsteps);`

Description The function IDASetMaxNumSteps specifies the maximum number of steps to be taken by the solver in its attempt to reach the next output time.

Arguments ida_mem (void *) pointer to the IDAS memory block.

mxsteps (long int) maximum allowed number of steps.

Return value The return value flag (of type int) is one of

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

Notes Passing mxsteps $= 0$ results in IDAS using the default value (500).

Passing mxsteps < 0 disables the test (*not recommended).*

IDASetInitStep

Call `flag = IDASetInitStep(ida_mem, hin);`

Description The function IDASetInitStep specifies the initial step size.

Arguments ida_mem (void *) pointer to the IDAS memory block.

hin (realtype) value of the initial step size to be attempted. Pass 0.0 to have IDAS use the default value.

Return value The return value flag (of type int) is one of

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

Notes By default, IDAS estimates the initial step as the solution of $\|h\dot{y}\|_{\mathrm{WRMS}} = 1/2$, with an added restriction that $|h| \leq .001|$tout - t0$|$.

IDASetMaxStep

Call `flag = IDASetMaxStep(ida_mem, hmax);`

Description The function IDASetMaxStep specifies the maximum absolute value of the step size.

Arguments ida_mem (void *) pointer to the IDAS memory block.

hmax (realtype) maximum absolute value of the step size.

Return value The return value flag (of type int) is one of

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

IDA_ILL_INPUT Either hmax is not positive or it is smaller than the minimum allowable step.

Notes Pass hmax$= 0$ to obtain the default value ∞.

`IDASetStopTime`

Call `flag = IDASetStopTime(ida_mem, tstop);`

Description The function `IDASetStopTime` specifies the value of the independent variable t past which the solution is not to proceed.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`tstop` (`realtype`) value of the independent variable past which the solution should not proceed.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT` The value of `tstop` is not beyond the current t value, t_n.

Notes The default, if this routine is not called, is that no stop time is imposed.

`IDASetMaxErrTestFails`

Call `flag = IDASetMaxErrTestFails(ida_mem, maxnef);`

Description The function `IDASetMaxErrTestFails` specifies the maximum number of error test failures in attempting one step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`maxnef` (`int`) maximum number of error test failures allowed on one step (> 0).

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 7.

`IDASetMaxNonlinIters`

Call `flag = IDASetMaxNonlinIters(ida_mem, maxcor);`

Description The function `IDASetMaxNonlinIters` specifies the maximum number of nonlinear solver iterations at one step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`maxcor` (`int`) maximum number of nonlinear solver iterations allowed on one step (> 0).

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 3.

`IDASetMaxConvFails`

Call `flag = IDASetMaxConvFails(ida_mem, maxncf);`

Description The function `IDASetMaxConvFails` specifies the maximum number of nonlinear solver convergence failures at one step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`maxncf` (`int`) maximum number of allowable nonlinear solver convergence failures on one step (> 0).

Return value The return value `flag` (of type `int`) is one of

IDA_SUCCESS The optional value has been successfully set.
IDA_MEM_NULL The ida_mem pointer is NULL.

Notes The default value is 10.

IDASetNonlinConvCoef

Call `flag = IDASetNonlinConvCoef(ida_mem, nlscoef);`

Description The function IDASetNonlinConvCoef specifies the safety factor in the nonlinear convergence test; see Chapter 2, Eq. (2.8).

Arguments ida_mem (void *) pointer to the IDAS memory block.
nlscoef (realtype) coefficient in nonlinear convergence test (> 0.0).

Return value The return value flag (of type int) is one of
IDA_SUCCESS The optional value has been successfully set.
IDA_MEM_NULL The ida_mem pointer is NULL.
IDA_ILL_INPUT The value of nlscoef is $<= 0.0$.

Notes The default value is 0.33.

IDASetSuppressAlg

Call `flag = IDASetSuppressAlg(ida_mem, suppressalg);`

Description The function IDASetSuppressAlg indicates whether or not to suppress algebraic variables in the local error test.

Arguments ida_mem (void *) pointer to the IDAS memory block.
suppressalg (booleantype) indicates whether to suppress (TRUE) or not (FALSE) the algebraic variables in the local error test.

Return value The return value flag (of type int) is one of
IDA_SUCCESS The optional value has been successfully set.
IDA_MEM_NULL The ida_mem pointer is NULL.

Notes The default value is FALSE.

If suppressalg=TRUE is selected, then the id vector must be set (through IDASetId) to specify the algebraic components.

In general, the use of this option (with suppressalg = TRUE) is *discouraged* when solving DAE systems of index 1, whereas it is generally *encouraged* for systems of index 2 or more. See pp. 146-147 of Ref. [3] for more on this issue.

IDASetId

Call `flag = IDASetId(ida_mem, id);`

Description The function IDASetId specifies algebraic/differential components in the y vector.

Arguments ida_mem (void *) pointer to the IDAS memory block.
id (N_Vector) state vector. A value of 1.0 indicates a differential variable, while 0.0 indicates an algebraic variable.

Return value The return value flag (of type int) is one of
IDA_SUCCESS The optional value has been successfully set.
IDA_MEM_NULL The ida_mem pointer is NULL.

Notes The vector id is required if the algebraic variables are to be suppressed from the local error test (see IDASetSuppressAlg) or if IDACalcIC is to be called with icopt = IDA_YA_YDP_INIT (see §4.5.4).

`IDASetConstraints`

Call `flag = IDASetConstraints(ida_mem, constraints);`

Description The function `IDASetConstraints` specifies a vector defining inequality constraints for each component of the solution vector y.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`constraints` (`N_Vector`) vector of constraint flags. If `constraints[i]` is

- 0.0 then no constraint is imposed on y_i.
- 1.0 then y_i will be constrained to be $y_i \geq 0.0$.
- −1.0 then y_i will be constrained to be $y_i \leq 0.0$.
- 2.0 then y_i will be constrained to be $y_i > 0.0$.
- −2.0 then y_i will be constrained to be $y_i < 0.0$.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	The constraints vector contains illegal values.

Notes The presence of a non-`NULL` constraints vector that is not 0.0 in all components will cause constraint checking to be performed. However, a call with 0.0 in all components of `constraints` will result in an illegal input return.

4.5.7.2 Dense/band direct linear solvers optional input functions

The IDADENSE solver needs a function to compute a dense approximation to the Jacobian matrix $J(t, y, \dot{y})$. This function must be of type `IDADlsDenseJacFn`. The user can supply his/her own dense Jacobian function, or use the default internal difference quotient approximation that comes with the IDADENSE solver. To specify a user-supplied Jacobian function `djac`, IDADENSE provides the function `IDADlsSetDenseJacFn`. The IDADENSE solver passes the pointer `user_data` to the dense Jacobian function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer `user_data` may be specified through `IDASetUserData`.

`IDADlsSetDenseJacFn`

Call `flag = IDADlsSetDenseJacFn(ida_mem, djac);`

Description The function `IDADlsSetDenseJacFn` specifies the dense Jacobian approximation function to be used.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`djac` (`IDADlsDenseJacFn`) user-defined dense Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS`	The optional value has been successfully set.
`IDADLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADLS_LMEM_NULL`	The IDADENSE linear solver has not been initialized.

Notes By default, IDADENSE uses an internal difference quotient function. If `NULL` is passed to `djac`, this default function is used.

The function type `IDADlsDenseJacFn` is described in §4.6.5.

The IDABAND solver needs a function to compute a banded approximation to the Jacobian matrix $J(t, y, \dot{y})$. This function must be of type `IDADlsBandJacFn`. The user can supply his/her own banded Jacobian approximation function, or use the default difference quotient function that comes with the IDABAND solver. To specify a user-supplied Jacobian function `bjac`, IDABAND provides the function

IDADlsSetBandJacFn. The IDABAND solver passes the pointer user_data to the banded Jacobian approximation function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer user_data may be specified through IDASetUserData.

IDADlsSetBandJacFn

Call `flag = IDADlsSetBandJacFn(ida_mem, bjac);`

Description The function IDADlsSetBandJacFn specifies the banded Jacobian approximation function to be used.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`bjac` (IDADlsBandJacFn) user-defined banded Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of

IDADLS_SUCCESS	The optional value has been successfully set.
IDADLS_MEM_NULL	The ida_mem pointer is NULL.
IDADLS_LMEM_NULL	The IDABAND linear solver has not been initialized.

Notes By default, IDABAND uses an internal difference quotient function. If NULL is passed to bjac, this default function is used.

The function type IDADlsBandJacFn is described in §4.6.6.

4.5.7.3 Sparse direct linear solvers optional input functions

The IDAKLU and IDASUPERLUMT solvers require a function to compute a compressed-sparse-column approximation ot the Jacobian matrix $J(t, y, \dot{y})$. This function must be of type IDASlsSparseJacFn. The user must supply a custom sparse Jacobian function since a difference quotient approximation would not leverage the underlying sparse matrix structure of the problem. To specify a user-supplied Jacobian function sjac, IDAKLU and IDASUPERLUMT provide the function IDASlsSetSparseJacFn. The IDAKLU and IDASUPERLUMT solvers pass the pointer user_data to the sparse Jacobian function. This mechanism allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer user_data may be specified through IDASetUserData.

IDASlsSetSparseJacFn

Call `flag = IDASlsSetSparseJacFn(ida_mem, sjac);`

Description The function IDASlsSetSparseJacFn specifies the sparse Jacobian approximation function to be used.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`sjac` (IDASlsSparseJacFn) user-defined sparse Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of

IDASLS_SUCCESS	The optional value has been successfully set.
IDASLS_MEM_NULL	The ida_mem pointer is NULL.
IDASLS_LMEM_NULL	The IDAKLU or IDASUPERLUMT linear solver has not been initialized.

Notes The function type IDASlsSparseJacFn is described in §4.6.7.

When using a sparse direct solver, there may be instances when the number of state variables does not change, but the number of nonzeroes in the Jacobian does change. In this case, for the IDAKLU solver, we provide the following reinitialization function. This function reinitializes the Jacobian matrix memory for the new number of nonzeroes and sets flags for a new factorization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed, or where the structure of the linear system has changed, requiring a new symbolic (and numeric) factorization.

`IDAKLUReInit`

Call `flag = IDAKLUReInit(ida_mem, n, nnz, reinit_type);`

Description The function `IDAKLUReInit` reinitializes Jacobian matrix memory and flags for new symbolic and numeric KLU factorizations.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`n` (`int`) number of state variables in the system.

`nnz` (`int`) number of nonzeroes in the Jacobian matrix.

`reinit_type` (`int`) type of reinitialization:

1. The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.
2. Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the prior call to IDAKLU.

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS` The reinitialization succeeded.

`IDASLS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASLS_LMEM_NULL` The IDAKLU linear solver has not been initialized.

`IDASLS_ILL_INPUT` The given `reinit_type` has an illegal value.

`IDASLS_MEM_FAIL` A memory allocation failed.

Notes The default value for `reinit_type` is 2.

Both the IDAKLU and IDASUPERLUMT solvers can apply reordering algorithms to minimize fill-in for the resulting sparse *LU* decomposition internal to the solver. The approximate minimal degree ordering for nonsymmetric matrices given by the `COLAMD` algorithm is the default algorithm used within both solvers, but alternate orderings may be chosen through one of the following two functions. The input values to these functinos are the numeric values used in the respective packages, and the user-supplied value will be passed directly to the package.

`IDAKLUSetOrdering`

Call `flag = IDAKLUSetOrdering(ida_mem, ordering_choice);`

Description The function `IDAKLUSetOrdering` specifies the ordering algorithm used by IDAKLU for reducing fill.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`ordering_choice` (`int`) flag denoting algorithm choice:

0 `AMD`

1 `COLAMD`

2 natural ordering

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS` The optional value has been successfully set.

`IDASLS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASLS_ILL_INPUT` The supplied value of `ordering_choice` is illegal.

Notes The default ordering choice is 1 for `COLAMD`.

`IDASuperLUMTSetOrdering`

Call `flag = IDASuperLUMTSetOrdering(ida_mem, ordering_choice);`

Description The function `IDASuperLUMTSetOrdering` specifies the ordering algorithm used by IDASUPERLUMT for reducing fill.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`ordering_choice` (`int`) flag denoting algorithm choice:
0 natural ordering
1 minimal degree ordering on $J^T J$
2 minimal degree ordering on $J^T + J$
3 `COLAMD`

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS`	The optional value has been successfully set.
`IDASLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASLS_ILL_INPUT`	The supplied value of `ordering_choice` is illegal.

Notes The default ordering choice is 3 for `COLAMD`.

4.5.7.4 Iterative linear solvers optional input functions

If preconditioning is to be done with one of the IDASPILS linear solvers, then the user must supply a preconditioner solve function `psolve` and specify its name through a call to `IDASpilsSetPreconditioner`. The evaluation and preprocessing of any Jacobian-related data needed by the user's preconditioner solve function is done in the optional user-supplied function `psetup`. Both of these functions are fully specified in §4.6. If used, the name of the `psetup` function should be specified in the call to `IDASpilsSetPreconditioner`.

The pointer `user_data` received through `IDASetUserData` (or a pointer to `NULL` if `user_data` was not specified) is passed to the preconditioner `psetup` and `psolve` functions. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied preconditioner functions without using global data in the program.

The IDASPILS solvers require a function to compute an approximation to the product between the Jacobian matrix $J(t, y)$ and a vector v. The user can supply his/her own Jacobian-times-vector approximation function, or use the default internal difference quotient function that comes with the IDASPILS solvers. A user-defined Jacobian-vector function must be of type `IDASpilsJacTimesVecFn` and can be specified through a call to `IDASpilsSetJacTimesVecFn` (see §4.6.8 for specification details). As with the preconditioner user-supplied functions, a pointer to the user-defined data structure, `user_data`, specified through `IDASetUserData` (or a `NULL` pointer otherwise) is passed to the Jacobian-times-vector function `jtimes` each time it is called.

`IDASpilsSetPreconditioner`

Call `flag = IDASpilsSetPreconditioner(ida_mem, psetup, psolve);`

Description The function `IDASpilsSetPreconditioner` specifies the preconditioner setup and solve functions.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`psetup` (`IDASpilsPrecSetupFn`) user-defined preconditioner setup function. Pass `NULL` if no setup is to be done.
`psolve` (`IDASpilsPrecSolveFn`) user-defined preconditioner solve function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional values have been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.

IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.

Notes The function type IDASpilsPrecSolveFn is described in §4.6.9. The function type IDASpilsPrecSetupFn is described in §4.6.10.

IDASpilsSetJacTimesVecFn

Call `flag = IDASpilsSetJacTimesVecFn(ida_mem, jtimes);`

Description The function IDASpilsSetJacTimesFn specifies the Jacobian-vector function to be used.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`jtimes` (IDASpilsJacTimesVecFn) user-defined Jacobian-vector product function.

Return value The return value `flag` (of type `int`) is one of

IDASPILS_SUCCESS The optional value has been successfully set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.

Notes By default, the IDASPILS solvers use the difference quotient function. If NULL is passed to jtimes, this default function is used.

The function type IDASpilsJacTimesVecFn is described in §4.6.8.

IDASpilsSetGSType

Call `flag = IDASpilsSetGSType(ida_mem, gstype);`

Description The function IDASpilsSetGSType specifies the Gram-Schmidt orthogonalization to be used. This must be one of the enumeration constants MODIFIED_GS or CLASSICAL_GS. These correspond to using modified Gram-Schmidt and classical Gram-Schmidt, respectively.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`gstype` (`int`) type of Gram-Schmidt orthogonalization.

Return value The return value `flag` (of type `int`) is one of

IDASPILS_SUCCESS The optional value has been successfully set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT The value of gstype is not valid.

Notes The default value is MODIFIED_GS.

This option is available only for the IDASPGMR linear solver.

IDASpilsSetMaxRestarts

Call `flag = IDASpilsSetMaxRestarts(ida_mem, maxrs);`

Description The function IDASpilsSetMaxRestarts specifies the maximum number of restarts to be used in the GMRES algorithm.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`maxrs` (`int`) maximum number of restarts.

Return value The return value `flag` (of type `int`) is one of

IDASPILS_SUCCESS The optional value has been successfully set.
IDASPILS_MEM_NULL The ida_mem pointer is NULL.
IDASPILS_LMEM_NULL The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT The maxrs argument is negative.

Notes The default value is 5. Pass `maxrs` = 0 to specify no restarts.

This option is available only for the IDASPGMR linear solver.

`IDASpilsSetEpsLin`

Call `flag = IDASpilsSetEpsLin(ida_mem, eplifac);`

Description The function `IDASpilsSetEpsLin` specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the Newton iteration test constant. (See §2.1).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`eplifac` (`realtype`) linear convergence safety factor (>= 0.0).

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_ILL_INPUT`	The value of `eplifac` is negative.

Notes The default value is 0.05.

Passing a value `eplifac`= 0.0 also indicates using the default value.

`IDASpilsSetIncrementFactor`

Call `flag = IDASpilsSetIncrementFactor(ida_mem, dqincfac);`

Description The function `IDASpilsSetIncrementFactor` specifies a factor in the increments to y used in the difference quotient approximations to the Jacobian-vector products. (See §2.1). The increment used to approximate Jv will be $\sigma =$ `dqincfac`$/\|v\|$.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`dqincfac` (`realtype`) difference quotient increment factor.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_ILL_INPUT`	The increment factor was non-positive.

Notes The default value is `dqincfac` = 1.0.

`IDASpilsSetMaxl`

Call `flag = IDASpilsSetMaxl(ida_mem, maxl);`

Description The function `IDASpilsSetMaxl` resets the maximum Krylov subspace dimension for the Bi-CGStab or TFQMR methods.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxl` (`int`) maximum dimension of the Krylov subspace.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes The maximum subspace dimension is initially specified in the call to the linear solver specification function (see §4.5.3). This function call is needed only if `maxl` is being changed from its previous value.

An input value `maxl` ≤ 0 will result in the default value, 5.

This option is available only for the IDASPBCG and IDASPTFQMR linear solvers.

4.5.7.5 Initial condition calculation optional input functions

The following functions can be called just prior to calling `IDACalcIC` to set optional inputs controlling the initial condition calculation.

`IDASetNonlinConvCoefIC`

Call `flag = IDASetNonlinConvCoefIC(ida_mem, epiccon);`

Description The function `IDASetNonlinConvCoefIC` specifies the positive constant in the Newton iteration convergence test within the initial condition calculation.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`epiccon` (`realtype`) coefficient in the Newton convergence test (> 0).

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	The `epiccon` factor is <= 0.0.

Notes The default value is $0.01 \cdot 0.33$.

This test uses a weighted RMS norm (with weights defined by the tolerances). For new initial value vectors y and $\dot{y}$ to be accepted, the norm of $J^{-1}F(t_0, y, \dot{y})$ must be $\leq$ `epiccon`, where J is the system Jacobian.

`IDASetMaxNumStepsIC`

Call `flag = IDASetMaxNumStepsIC(ida_mem, maxnh);`

Description The function `IDASetMaxNumStepsIC` specifies the maximum number of steps allowed when `icopt`=`IDA_YA_YDP_INIT` in `IDACalcIC`, where h appears in the system Jacobian, $J = \partial F/\partial y + (1/h)\partial F/\partial \dot{y}$.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxnh` (`int`) maximum allowed number of values for h.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	`maxnh` is non-positive.

Notes The default value is 5.

`IDASetMaxNumJacsIC`

Call `flag = IDASetMaxNumJacsIC(ida_mem, maxnj);`

Description The function `IDASetMaxNumJacsIC` specifies the maximum number of the approximate Jacobian or preconditioner evaluations allowed when the Newton iteration appears to be slowly converging.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxnj` (`int`) maximum allowed number of Jacobian or preconditioner evaluations.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_ILL_INPUT` `maxnj` is non-positive.

Notes The default value is 4.

`IDASetMaxNumItersIC`

Call `flag = IDASetMaxNumItersIC(ida_mem, maxnit);`

Description The function `IDASetMaxNumItersIC` specifies the maximum number of Newton iterations allowed in any one attempt to solve the initial conditions calculation problem.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxnit` (`int`) maximum number of Newton iterations.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_ILL_INPUT` `maxnit` is non-positive.

Notes The default value is 10.

`IDASetMaxBacksIC`

Call `flag = IDASetMaxBacksIC(ida_mem, maxbacks);`

Description The function `IDASetMaxBacksIC` specifies the maximum number of linesearch backtracks allowed in any Newton iteration, when solving the initial conditions calculation problem.

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.

`maxbacks` (`int`) maximum number of linesearch backtracks per Newton step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_ILL_INPUT` `maxbacks` is non-positive.

Notes The default value is 100.

If `IDASetMaxBacksIC` is called in a Forward Sensitivity Analysis, the the limit `maxbacks` applies in the calculation of both the initial state values and the initial sensititivies.

`IDASetLineSearchOffIC`

Call `flag = IDASetLineSearchOffIC(ida_mem, lsoff);`

Description The function `IDASetLineSearchOffIC` specifies whether to turn on or off the linesearch algorithm.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`lsoff` (`booleantype`) a flag to turn off (`TRUE`) or keep (`FALSE`) the linesearch algorithm.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is `FALSE`.

`IDASetStepToleranceIC`

Call `flag = IDASetStepToleranceIC(ida_mem, steptol);`

Description The function `IDASetStepToleranceIC` specifies a positive lower bound on the Newton step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`steptol` (`int`) Minimum allowed WRMS-norm of the Newton step (> 0.0).

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	The `steptol` tolerance is $<= 0.0$.

Notes The default value is (unit roundoff)$^{2/3}$.

4.5.7.6 Rootfinding optional input functions

The following functions can be called to set optional inputs to control the rootfinding algorithm.

`IDASetRootDirection`

Call `flag = IDASetRootDirection(ida_mem, rootdir);`

Description The function `IDASetRootDirection` specifies the direction of zero-crossings to be located and returned to the user.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`rootdir` (`int *`) state array of length `nrtfn`, the number of root functions g_i, as specified in the call to the function `IDARootInit`. A value of 0 for `rootdir[i]` indicates that crossing in either direction should be reported for g_i. A value of $+1$ or -1 indicates that the solver should report only zero-crossings where g_i is increasing or decreasing, respectively.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	rootfinding has not been activated through a call to `IDARootInit`.

Notes The default behavior is to locate both zero-crossing directions.

`IDASetNoInactiveRootWarn`

Call `flag = IDASetNoInactiveRootWarn(ida_mem);`

Description The function `IDASetNoInactiveRootWarn` disables issuing a warning if some root function appears to be identically zero at the beginning of the integration.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

Notes IDAS will not report the initial conditions as a possible zero-crossing (assuming that one or more components g_i are zero at the initial time). However, if it appears that some g_i is identically zero at the initial time (i.e., g_i is zero at the initial time and after the first step), IDAS will issue a warning which can be disabled with this optional input function.

4.5.8 Interpolated output function

An optional function IDAGetDky is available to obtain additional output values. This function must be called after a successful return from IDASolve and provides interpolated values of y or its derivatives of order up to the last internal order used for any value of t in the last internal step taken by IDAS.

The call to the IDAGetDky function has the following form:

IDAGetDky

Call `flag = IDAGetDky(ida_mem, t, k, dky);`

Description The function IDAGetDky computes the interpolated values of the k^{th} derivative of y for any value of t in the last internal step taken by IDAS. The value of k must be non-negative and smaller than the last internal order used. A value of 0 for k means that the y is interpolated. The value of t must satisfy $t_n - h_u \leq t \leq t_n$, where t_n denotes the current internal time reached, and h_u is the last internal step size used successfully.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `t` (`realtype`) time at which to interpolate.
- `k` (`int`) integer specifying the order of the derivative of y wanted.
- `dky` (`N_Vector`) vector containing the interpolated k^{th} derivative of $y(t)$.

Return value The return value `flag` (of type `int`) is one of

IDA_SUCCESS	IDAGetDky succeeded.
IDA_MEM_NULL	The ida_mem argument was NULL.
IDA_BAD_T	t is not in the interval $[t_n - h_u, t_n]$.
IDA_BAD_K	k is not one of $\{0, 1, \ldots, klast\}$.
IDA_BAD_DKY	dky is NULL.

Notes It is only legal to call the function IDAGetDky after a successful return from IDASolve. Functions IDAGetCurrentTime, IDAGetLastStep and IDAGetLastOrder (see §4.5.9.2) can be used to access t_n, h_u and $klast$.

4.5.9 Optional output functions

IDAS provides an extensive list of functions that can be used to obtain solver performance information. Table 4.3 lists all optional output functions in IDAS, which are then described in detail in the remainder of this section.

Some of the optional outputs, especially the various counters, can be very useful in determining how successful the IDAS solver is in doing its job. For example, the counters `nsteps` and `nrevals` provide a rough measure of the overall cost of a given run, and can be compared among runs with differing input options to suggest which set of options is most efficient. The ratio `nniters/nsteps` measures the performance of the Newton iteration in solving the nonlinear systems at each time step; typical values for this range from 1.1 to 1.8. The ratio `njevals/nniters` (in the case of a direct linear solver), and the ratio `npevals/nniters` (in the case of an iterative linear solver) measure the overall degree of nonlinearity in these systems, and also the quality of the approximate Jacobian or preconditioner being used. Thus, for example, `njevals/nniters` can indicate if a user-supplied Jacobian is inaccurate, if this ratio is larger than for the case of the corresponding internal Jacobian. The ratio `nliters/nniters` measures the performance of the Krylov iterative linear solver, and thus (indirectly) the quality of the preconditioner.

4.5.9.1 SUNDIALS version information

The following functions provide a way to get SUNDIALS version information at runtime.

Table 4.3: Optional outputs from IDAS, IDADLS, IDASLS, and IDASPILS

Optional output	Function name
IDAS main solver	
Size of IDAS real and integer workspace	IDAGetWorkSpace
Cumulative number of internal steps	IDAGetNumSteps
No. of calls to residual function	IDAGetNumResEvals
No. of calls to linear solver setup function	IDAGetNumLinSolvSetups
No. of local error test failures that have occurred	IDAGetNumErrTestFails
Order used during the last step	IDAGetLastOrder
Order to be attempted on the next step	IDAGetCurrentOrder
Order reductions due to stability limit detection	IDAGetNumStabLimOrderReds
Actual initial step size used	IDAGetActualInitStep
Step size used for the last step	IDAGetLastStep
Step size to be attempted on the next step	IDAGetCurrentStep
Current internal time reached by the solver	IDAGetCurrentTime
Suggested factor for tolerance scaling	IDAGetTolScaleFactor
Error weight vector for state variables	IDAGetErrWeights
Estimated local errors	IDAGetEstLocalErrors
No. of nonlinear solver iterations	IDAGetNumNonlinSolvIters
No. of nonlinear convergence failures	IDAGetNumNonlinSolvConvFails
Array showing roots found	IDAGetRootInfo
No. of calls to user root function	IDAGetNumGEvals
Name of constant associated with a return flag	IDAGetReturnFlagName
IDAS initial conditions calculation	
Number of backtrack operations	IDAGetNumBacktrackops
Corrected initial conditions	IDAGetConsistentIC
IDADLS linear solver	
Size of real and integer workspace	IDADlsGetWorkSpace
No. of Jacobian evaluations	IDADlsGetNumJacEvals
No. of residual calls for finite diff. Jacobian evals.	IDADlsGetNumResEvals
Last return from a linear solver function	IDADlsGetLastFlag
Name of constant associated with a return flag	IDADlsGetReturnFlagName
IDASLS linear solver	
No. of Jacobian evaluations	IDASlsGetNumJacEvals
Last return from a linear solver function	IDASlsGetLastFlag
Name of constant associated with a return flag	IDASlsGetReturnFlagName
IDASPILS linear solvers	
Size of real and integer workspace	IDASpilsGetWorkSpace
No. of linear iterations	IDASpilsGetNumLinIters
No. of linear convergence failures	IDASpilsGetNumConvFails
No. of preconditioner evaluations	IDASpilsGetNumPrecEvals
No. of preconditioner solves	IDASpilsGetNumPrecSolves
No. of Jacobian-vector product evaluations	IDASpilsGetNumJtimesEvals
No. of residual calls for finite diff. Jacobian-vector evals.	IDASpilsGetNumResEvals
Last return from a linear solver function	IDASpilsGetLastFlag
Name of constant associated with a return flag	IDASpilsGetReturnFlagName

`SUNDIALSGetVersion`

Call `flag = SUNDIALSGetVersion(version, len);`

Description The function `SUNDIALSGetVersion` fills a string with SUNDIALS version information.

Arguments `version` (`char *`) string to hold the SUNDIALS version information.
`len` (`int`) length of `version`.

Return value If successful, `SUNDIALSGetVersion` returns 0 and `version` contains the SUNDIALS version information. Otherwise, it returns -1 and `version` is not set.

Notes A string of 25 characters should be sufficient to hold the version information.

`SUNDIALSGetVersionNumber`

Call `flag = SUNDIALSGetVersionNumber(&major, &minor, &patch, label, length);`

Description The function `SUNDIALSGetVersionNumber` set integers for the SUNDIALS major, minor, and patch release numbers and fills a string with the release label if applicable.

Arguments `major` (`int`) SUNDIALS release major version number
`minor` (`int`) SUNDIALS release minor version number
`patch` (`int`) SUNDIALS release patch version number
`label` (`char *`) string to hold the SUNDIALS release label
`len` (`int`) length of `label`

Return value If successful, `SUNDIALSGetVersion` returns 0 and the `major`, `minor`, `patch`, and `label` values are set. Otherwise, it returns -1 and the values are not set.

Notes A string of 10 characters should be sufficient to hold the label information. If a label is not used in the release version, an empty string is returned in `label`.

4.5.9.2 Main solver optional output functions

IDAS provides several user-callable functions that can be used to obtain different quantities that may be of interest to the user, such as solver workspace requirements, solver performance statistics, as well as additional data from the IDAS memory block (a suggested tolerance scaling factor, the error weight vector, and the vector of estimated local errors). Also provided are functions to extract statistics related to the performance of the IDAS nonlinear solver being used. As a convenience, additional extraction functions provide the optional outputs in groups. These optional output functions are described next.

`IDAGetWorkSpace`

Call `flag = IDAGetWorkSpace(ida_mem, &lenrw, &leniw);`

Description The function `IDAGetWorkSpace` returns the IDAS real and integer workspace sizes.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`lenrw` (`long int`) number of real values in the IDAS workspace.
`leniw` (`long int`) number of integer values in the IDAS workspace.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes In terms of the problem size N, the maximum method order `maxord`, and the number `nrtfn` of root functions (see §4.5.5), the actual size of the real workspace, in `realtype` words, is given by the following:

- base value: `lenrw` $= 55 + (m + 6) * N_r + 3*$`nrtfn`;

- with `IDASVtolerances`: `lenrw` = `lenrw` $+N_r$;
- with constraint checking (see `IDASetConstraints`): `lenrw` = `lenrw` $+N_r$;
- with `id` specified (see `IDASetId`): `lenrw` = `lenrw` $+N_r$;

where $m = \max(\texttt{maxord}, 3)$, and N_r is the number of real words in one `N_Vector` ($\approx N$).

The size of the integer workspace (without distinction between `int` and `long int` words) is given by:

- base value: `leniw` = $38 + (m + 6) * N_i$ + `nrtfn`;
- with `IDASVtolerances`: `leniw` = `leniw` $+N_i$;
- with constraint checking: `lenrw` = `lenrw` $+N_i$;
- with `id` specified: `lenrw` = `lenrw` $+N_i$;

where N_i is the number of integer words in one `N_Vector` (= 1 for NVECTOR_SERIAL and 2*`npes` for NVECTOR_PARALLEL on `npes` processors).

For the default value of `maxord`, with no rootfinding, no `id`, no constraints, and with no call to `IDASVtolerances`, these lengths are given roughly by: `lenrw` = $55 + 11N$, `leniw` = 49.

Note that additional memory is allocated if quadratures and/or forward sensitivity integration is enabled. See §4.7.1 and §5.2.1 for more details.

`IDAGetNumSteps`

Call `flag = IDAGetNumSteps(ida_mem, &nsteps);`

Description The function `IDAGetNumSteps` returns the cumulative number of internal steps taken by the solver (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nsteps` (`long int`) number of steps taken by IDAS.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetNumResEvals`

Call `flag = IDAGetNumResEvals(ida_mem, &nrevals);`

Description The function `IDAGetNumResEvals` returns the number of calls to the user's residual evaluation function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nrevals` (`long int`) number of calls to the user's `res` function.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The `nrevals` value returned by `IDAGetNumResEvals` does not account for calls made to `res` from a linear solver or preconditioner module.

`IDAGetNumLinSolvSetups`

Call `flag = IDAGetNumLinSolvSetups(ida_mem, &nlinsetups);`

Description The function `IDAGetNumLinSolvSetups` returns the cumulative number of calls made to the linear solver's setup function (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nlinsetups` (`long int`) number of calls made to the linear solver setup function.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetNumErrTestFails`

Call `flag = IDAGetNumErrTestFails(ida_mem, &netfails);`

Description The function `IDAGetNumErrTestFails` returns the cumulative number of local error test failures that have occurred (total so far).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`netfails` (`long int`) number of error test failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetLastOrder`

Call `flag = IDAGetLastOrder(ida_mem, &klast);`

Description The function `IDAGetLastOrder` returns the integration method order used during the last internal step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`klast` (`int`) method order used on the last internal step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetCurrentOrder`

Call `flag = IDAGetCurrentOrder(ida_mem, &kcur);`

Description The function `IDAGetCurrentOrder` returns the integration method order to be used on the next internal step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`kcur` (`int`) method order to be used on the next internal step.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetLastStep`

Call `flag = IDAGetLastStep(ida_mem, &hlast);`

Description The function `IDAGetLastStep` returns the integration step size taken on the last internal step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`hlast` (`realtype`) step size taken on the last internal step by IDA, or last artificial step size used in `IDACalcIC`, whichever was called last.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetCurrentStep`

Call `flag = IDAGetCurrentStep(ida_mem, &hcur);`

Description The function `IDAGetCurrentStep` returns the integration step size to be attempted on the next internal step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`hcur` (`realtype`) step size to be attempted on the next internal step.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetActualInitStep`

Call `flag = IDAGetActualInitStep(ida_mem, &hinused);`

Description The function `IDAGetActualInitStep` returns the value of the integration step size used on the first step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`hinused` (`realtype`) actual value of initial step size.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes Even if the value of the initial integration step size was specified by the user through a call to `IDASetInitStep`, this value might have been changed by IDAS to ensure that the step size is within the prescribed bounds ($h_{\min} \le h_0 \le h_{\max}$), or to meet the local error test.

`IDAGetCurrentTime`

Call `flag = IDAGetCurrentTime(ida_mem, &tcur);`

Description The function `IDAGetCurrentTime` returns the current internal time reached by the solver.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`tcur` (`realtype`) current internal time reached.

Return value The return value `flag` (of type `int`) is one of
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetTolScaleFactor`

Call `flag = IDAGetTolScaleFactor(ida_mem, &tolsfac);`

Description The function `IDAGetTolScaleFactor` returns a suggested factor by which the user's tolerances should be scaled when too much accuracy has been requested for some internal step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`tolsfac` (`realtype`) suggested scaling factor for user tolerances.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetErrWeights`

Call `flag = IDAGetErrWeights(ida_mem, eweight);`

Description The function `IDAGetErrWeights` returns the solution error weights at the current time. These are the W_i given by Eq. (2.7) (or by the user's `IDAEwtFn`).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`eweight` (`N_Vector`) solution error weights at the current time.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The user must allocate space for `eweight`.

`IDAGetEstLocalErrors`

Call `flag = IDAGetEstLocalErrors(ida_mem, ele);`

Description The function `IDAGetEstLocalErrors` returns the estimated local errors.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`ele` (`N_Vector`) estimated local errors at the current time.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The user must allocate space for `ele`.
The values returned in `ele` are only valid if `IDASolve` returned a non-negative value.

The `ele` vector, togther with the `eweight` vector from `IDAGetErrWeights`, can be used to determine how the various components of the system contributed to the estimated local error test. Specifically, that error test uses the RMS norm of a vector whose components are the products of the components of these two vectors. Thus, for example, if there were recent error test failures, the components causing the failures are those with largest values for the products, denoted loosely as `eweight[i]*ele[i]`.

`IDAGetIntegratorStats`

Call
```
flag = IDAGetIntegratorStats(ida_mem, &nsteps, &nrevals, &nlinsetups,
                             &netfails, &klast, &kcur, &hinused,
                             &hlast, &hcur, &tcur);
```

Description The function `IDAGetIntegratorStats` returns the IDAS integrator statistics as a group.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`nsteps`	(`long int`) cumulative number of steps taken by IDAS.
`nrevals`	(`long int`) cumulative number of calls to the user's `res` function.
`nlinsetups`	(`long int`) cumulative number of calls made to the linear solver setup function.
`netfails`	(`long int`) cumulative number of error test failures.
`klast`	(`int`) method order used on the last internal step.
`kcur`	(`int`) method order to be used on the next internal step.
`hinused`	(`realtype`) actual value of initial step size.
`hlast`	(`realtype`) step size taken on the last internal step.
`hcur`	(`realtype`) step size to be attempted on the next internal step.
`tcur`	(`realtype`) current internal time reached.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	the optional output values have been successfully set.
`IDA_MEM_NULL`	the `ida_mem` pointer is `NULL`.

`IDAGetNumNonlinSolvIters`

Call `flag = IDAGetNumNonlinSolvIters(ida_mem, &nniters);`

Description The function `IDAGetNumNonlinSolvIters` returns the cumulative number of nonlinear (functional or Newton) iterations performed.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory block.
`nniters`	(`long int`) number of nonlinear iterations performed.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetNumNonlinSolvConvFails`

Call `flag = IDAGetNumNonlinSolvConvFails(ida_mem, &nncfails);`

Description The function `IDAGetNumNonlinSolvConvFails` returns the cumulative number of nonlinear convergence failures that have occurred.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory block.
`nncfails`	(`long int`) number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetNonlinSolvStats`

Call `flag = IDAGetNonlinSolvStats(ida_mem, &nniters, &nncfails);`

Description The function `IDAGetNonlinSolvStats` returns the IDAS nonlinear solver statistics as a group.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory block.
`nniters`	(`long int`) cumulative number of nonlinear iterations performed.
`nncfails`	(`long int`) cumulative number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.

`IDAGetReturnFlagName`

Call `name = IDAGetReturnFlagName(flag);`

Description The function `IDAGetReturnFlagName` returns the name of the IDAS constant corresponding to `flag`.

Arguments The only argument, of type `int`, is a return flag from an IDAS function.

Return value The return value is a string containing the name of the corresponding constant.

4.5.9.3 Initial condition calculation optional output functions

`IDAGetNumBcktrackOps`

Call `flag = IDAGetNumBacktrackOps(ida_mem, &nbacktr);`

Description The function `IDAGetNumBacktrackOps` returns the number of backtrack operations done in the linesearch algorithm in `IDACalcIC`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nbacktr` (`long int`) the cumulative number of backtrack operations.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDAGetConsistentIC`

Call `flag = IDAGetConsistentIC(ida_mem, yy0_mod, yp0_mod);`

Description The function `IDAGetConsistentIC` returns the corrected initial conditions calculated by `IDACalcIC`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`yy0_mod` (`N_Vector`) consistent solution vector.
`yp0_mod` (`N_Vector`) consistent derivative vector.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_ILL_INPUT` The function was not called before the first call to `IDASolve`.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes If the consistent solution vector or consistent derivative vector is not desired, pass `NULL` for the corresponding argument.

The user must allocate space for `yy0_mod` and `yp0_mod` (if not `NULL`).

4.5.9.4 Rootfinding optional output functions

There are two optional output functions associated with rootfinding.

`IDAGetRootInfo`

Call `flag = IDAGetRootInfo(ida_mem, rootsfound);`

Description The function `IDAGetRootInfo` returns an array showing which functions were found to have a root.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`rootsfound` (`int *`) array of length `nrtfn` with the indices of the user functions g_i found to have a root. For $i = 0, \ldots,$`nrtfn` -1, `rootsfound`$[i] \neq 0$ if g_i has a root, and $= 0$ if not.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output values have been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes Note that, for the components g_i for which a root was found, the sign of `rootsfound`$[i]$ indicates the direction of zero-crossing. A value of $+1$ indicates that g_i is increasing, while a value of -1 indicates a decreasing g_i.

The user must allocate memory for the vector `rootsfound`.

`IDAGetNumGEvals`

Call `flag = IDAGetNumGEvals(ida_mem, &ngevals);`

Description The function `IDAGetNumGEvals` returns the cumulative number of calls to the user root function g.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`ngevals` (`long int`) number of calls to the user's function `g` so far.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` The optional output value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

4.5.9.5 Dense/band direct linear solvers optional output functions

The following optional outputs are available from the IDADLS modules: workspace requirements, number of calls to the Jacobian routine, number of calls to the residual routine for finite-difference Jacobian approximation, and last return value from an IDADLS function. Note that, where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix `LS` (for Linear Solver) has been added here (e.g. `lenrwLS`).

`IDADlsGetWorkSpace`

Call `flag = IDADlsGetWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDADlsGetWorkSpace` returns the sizes of the real and integer workspaces used by an IDADLS linear solver (IDADENSE or IDABAND).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`lenrwLS` (`long int`) the number of real values in the IDADLS workspace.

`leniwLS` (`long int`) the number of integer values in the IDADLS workspace.

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS` The optional output value has been successfully set.

`IDADLS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDADLS_LMEM_NULL` The IDADLS linear solver has not been initialized.

Notes For the IDADENSE linear solver, in terms of the problem size N, the actual size of the real workspace is $2N^2$ `realtype` words, while the actual size of the integer workspace is N integer words. For the IDABAND linear solver, in terms of N and Jacobian half-bandwidths, the actual size of the real workspace is N (2 `mupper`+3 `mlower` +2) `realtype` words, while the actual size of the integer workspace is N integer words.

`IDADlsGetNumJacEvals`

Call `flag = IDADlsGetNumJacEvals(ida_mem, &njevals);`

Description The function `IDADlsGetNumJacEvals` returns the cumulative number of calls to the IDADLS (dense or banded) Jacobian approximation function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`njevals` (`long int`) the cumulative number of calls to the Jacobian function (total so far).

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS`	The optional output value has been successfully set.
`IDADLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADLS_LMEM_NULL`	The IDADENSE linear solver has not been initialized.

`IDADlsGetNumResEvals`

Call `flag = IDADlsGetNumResEvals(ida_mem, &nrevalsLS);`

Description The function `IDADlsGetNumResEvals` returns the cumulative number of calls to the user residual function due to the finite difference (dense or band) Jacobian approximation.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS`	The optional output value has been successfully set.
`IDADLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADLS_LMEM_NULL`	The IDADENSE linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if the default internal difference quotient function is used.

`IDADlsGetLastFlag`

Call `flag = IDADlsGetLastFlag(ida_mem, &lsflag);`

Description The function `IDADlsGetLastFlag` returns the last return value from an IDADLS routine.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`lsflag` (`long int`) the value of the last return flag from an IDADLS function.

Return value The return value `flag` (of type `int`) is one of

`IDADLS_SUCCESS`	The optional output value has been successfully set.
`IDADLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDADLS_LMEM_NULL`	The IDADENSE linear solver has not been initialized.

Notes If the IDADENSE setup function failed (i.e., `IDASolve` returned `IDA_LSETUP_FAIL`), the value `lsflag` is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the (dense or band) Jacobian matrix. For all other failures, the value of `lsflag` is negative.

`IDADlsGetReturnFlagName`

Call `name = IDADlsGetReturnFlagName(lsflag);`

Description The function `IDADlsGetReturnFlagName` returns the name of the IDADLS constant corresponding to `lsflag`.

Arguments The only argument, of type `long int`, is a return flag from an IDADLS function.

Return value The return value is a string containing the name of the corresponding constant. If $1 \leq$ `lsflag` $\leq N$ (LU factorization failed), this function returns "NONE".

4.5.9.6 Sparse direct linear solvers optional output functions

The following optional outputs are available from the IDASLS modules: number of calls to the Jacobian routine and last return value from an IDASLS function.

`IDASlsGetNumJacEvals`

Call `flag = IDASlsGetNumJacEvals(ida_mem, &njevals);`

Description The function `IDASlsGetNumJacEvals` returns the cumulative number of calls to the IDASLS sparse Jacobian approximation function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`njevals` (`long int`) the cumulative number of calls to the Jacobian function (total so far).

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS`	The optional output value has been successfully set.
`IDASLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASLS_LMEM_NULL`	The IDASLS linear solver has not been initialized.

`IDASlsGetLastFlag`

Call `flag = IDASlsGetLastFlag(ida_mem, &lsflag);`

Description The function `IDASlsGetLastFlag` returns the last return value from an IDASLS routine.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`lsflag` (`long int`) the value of the last return flag from an IDASLS function.

Return value The return value `flag` (of type `int`) is one of

`IDASLS_SUCCESS`	The optional output value has been successfully set.
`IDASLS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASLS_LMEM_NULL`	The IDASLS linear solver has not been initialized.

Notes

`IDASlsGetReturnFlagName`

Call `name = IDASlsGetReturnFlagName(lsflag);`

Description The function `IDASlsGetReturnFlagName` returns the name of the IDASLS constant corresponding to `lsflag`.

Arguments The only argument, of type `long int`, is a return flag from an IDASLS function.

Return value The return value is a string containing the name of the corresponding constant.

4.5.9.7 Iterative linear solvers optional output functions

The following optional outputs are available from the IDASPILS modules: workspace requirements, number of linear iterations, number of linear convergence failures, number of calls to the preconditioner setup and solve routines, number of calls to the Jacobian-vector product routine, number of calls to the residual routine for finite-difference Jacobian-vector product approximation, and last return value from a linear solver function. Note that, where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix `LS` (for Linear Solver) has been added here (e.g. `lenrwLS`).

`IDASpilsGetWorkSpace`

Call `flag = IDASpilsGetWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDASpilsGetWorkSpace` returns the global sizes of the IDASPILS real and integer workspaces.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`lenrwLS` (`long int`) global number of real values in the IDASPILS workspace.
`leniwLS` (`long int`) global number of integer values in the IDASPILS workspace.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes In terms of the problem size N and maximum subspace size `maxl`, the actual size of the real workspace is roughly:
$N *$ (`maxl` $+5)+$ `maxl` $*($ `maxl` $+4) + 1$ `realtype` words for IDASPGMR,
$10 * N$ `realtype` words for IDASPBCG,
and $13 * N$ `realtype` words for IDASPTFQMR.

In a parallel setting, the above values are global, summed over all processors.

`IDASpilsGetNumLinIters`

Call `flag = IDASpilsGetNumLinIters(ida_mem, &nliters);`

Description The function `IDASpilsGetNumLinIters` returns the cumulative number of linear iterations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nliters` (`long int`) the current number of linear iterations.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumConvFails`

Call `flag = IDASpilsGetNumConvFails(ida_mem, &nlcfails);`

Description The function `IDASpilsGetNumConvFails` returns the cumulative number of linear convergence failures.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nlcfails` (`long int`) the current number of linear convergence failures.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumPrecEvals`

Call `flag = IDASpilsGetNumPrecEvals(ida_mem, &npevals);`

Description The function `IDASpilsGetNumPrecEvals` returns the cumulative number of preconditioner evaluations, i.e., the number of calls made to `psetup`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`npevals` (`long int`) the cumulative number of calls to `psetup`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumPrecSolves`

Call `flag = IDASpilsGetNumPrecSolves(ida_mem, &npsolves);`

Description The function `IDASpilsGetNumPrecSolves` returns the cumulative number of calls made to the preconditioner solve function, `psolve`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`npsolves` (`long int`) the cumulative number of calls to `psolve`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumJtimesEvals`

Call `flag = IDASpilsGetNumJtimesEvals(ida_mem, &njvevals);`

Description The function `IDASpilsGetNumJtimesEvals` returns the cumulative number of calls made to the Jacobian-vector function, `jtimes`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`njvevals` (`long int`) the cumulative number of calls to `jtimes`.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

`IDASpilsGetNumResEvals`

Call `flag = IDASpilsGetNumResEvals(ida_mem, &nrevalsLS);`

Description The function `IDASpilsGetNumResEvals` returns the cumulative number of calls to the user residual function for finite difference Jacobian-vector product approximation.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional output value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if the default `IDASpilsDQJtimes` difference quotient function is used.

`IDASpilsGetLastFlag`

Call `flag = IDASpilsGetLastFlag(ida_mem, &lsflag);`

Description The function `IDASpilsGetLastFlag` returns the last return value from an IDASPILS routine.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`lsflag` (`long int`) the value of the last return flag from an IDASPILS function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional output value has been successfully set.

`IDASPILS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDASPILS_LMEM_NULL` The IDASPILS linear solver has not been initialized.

Notes If the IDASPILS setup function failed (`IDASolve` returned `IDA_LSETUP_FAIL`), `lsflag` will be `SPGMR_PSET_FAIL_UNREC`, `SPBCG_PSET_FAIL_UNREC`, or `SPTFQMR_PSET_FAIL_UNREC`.

If the IDASPGMR solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `lsflag` contains the error return flag from `SpgmrSolve` and will be one of: `SPGMR_MEM_NULL`, indicating that the SPGMR memory is `NULL`; `SPGMR_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J * v$ function; `SPGMR_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably; `SPGMR_GS_FAIL`, indicating a failure in the Gram-Schmidt procedure; or `SPGMR_QRSOL_FAIL`, indicating that the matrix R was found to be singular during the QR solve phase.

If the IDASPBCG solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `lsflag` contains the error return flag from `SpbcgSolve` and will be one of: `SPBCG_MEM_NULL`, indicating that the SPBCGS memory is `NULL`; `SPBCG_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J*v$ function; or `SPBCG_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably.

If the IDASPTFQMR solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `lsflag` contains the error flag from `SptfqmrSolve` and will be one of: `SPTFQMR_MEM_NULL`, indicating that the SPTFQMR memory is `NULL`; `SPTFQMR_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J*v$ function; or `SPTFQMR_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably.

`IDASpilsGetReturnFlagName`

Call `name = IDASpilsGetReturnFlagName(lsflag);`

Description The function `IDASpilsGetReturnFlagName` returns the name of the IDASPILS constant corresponding to `lsflag`.

Arguments The only argument, of type `long int`, is a return flag from an IDASPILS function.

Return value The return value is a string containing the name of the corresponding constant.

4.5.10 IDAS reinitialization function

The function `IDAReInit` reinitializes the main IDAS solver for the solution of a new problem, where a prior call to `IDAInit` has been made. The new problem must have the same size as the previous one. `IDAReInit` performs the same input checking and initializations that `IDAInit` does, but does no memory allocation, as it assumes that the existing internal memory is sufficient for the new problem. A call to `IDAReInit` deletes the solution history that was stored internally during the previous integration. Following a successful call to `IDAReInit`, call `IDASolve` again for the solution of the new problem.

The use of `IDAReInit` requires that the maximum method order, `maxord`, is no larger for the new problem than for the problem specified in the last call to `IDAInit`. In addition, the same NVECTOR module set for the previous problem will be reused for the new problem.

If there are changes to the linear solver specifications, make the appropriate `IDA***` calls, as described in §4.5.3. If there are changes to any optional inputs, make the appropriate `IDASet***` calls, as described in §4.5.7. Otherwise, all solver inputs set previously remain in effect.

One important use of the `IDAReInit` function is in the treating of jump discontinuities in the residual function. Except in cases of fairly small jumps, it is usually more efficient to stop at each point of discontinuity and restart the integrator with a readjusted DAE model, using a call to `IDAReInit`. To stop when the location of the discontinuity is known, simply make that location a value of tout. To stop when the location of the discontinuity is determined by the solution, use the rootfinding feature. In either case, it is critical that the residual function *not* incorporate the discontinuity, but rather have a smooth extention over the discontinuity, so that the step across it (and subsequent rootfinding, if used) can be done efficiently. Then use a switch within the residual function (communicated through `user_data`) that can be flipped between the stopping of the integration and the restart, so that the restarted problem uses the new values (which have jumped). Similar comments apply if there is to be a jump in the dependent variable vector.

`IDAReInit`

Call `flag = IDAReInit(ida_mem, t0, y0, yp0);`

Description The function `IDAReInit` provides required problem specifications and reinitializes IDAS.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `t0` (`realtype`) is the initial value of t.
- `y0` (`N_Vector`) is the initial value of y.
- `yp0` (`N_Vector`) is the initial value of $\dot{y}$.

Return value The return value `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAReInit` was successful.
- `IDA_MEM_NULL` The IDAS memory block was not initialized through a previous call to `IDACreate`.
- `IDA_NO_MALLOC` Memory space for the IDAS memory block was not allocated through a previous call to `IDAInit`.
- `IDA_ILL_INPUT` An input argument to `IDAReInit` has an illegal value.

Notes If an error occurred, `IDAReInit` also sends an error message to the error handler function.

4.6 User-supplied functions

The user-supplied functions consist of one function defining the DAE residual, (optionally) a function that handles error and warning messages, (optionally) a function that provides the error weight vector, (optionally) a function that provides Jacobian-related information for the linear solver (if Newton iteration is chosen), and (optionally) one or two functions that define the preconditioner for use in any of the Krylov iteration algorithms.

4.6.1 Residual function

The user must provide a function of type `IDAResFn` defined as follows:

`IDAResFn`

Definition
```
typedef int (*IDAResFn)(realtype tt, N_Vector yy, N_Vector yp,
                        N_Vector rr, void *user_data);
```

Purpose This function computes the problem residual for given values of the independent variable t, state vector y, and derivative $\dot{y}$.

Arguments `tt` is the current value of the independent variable.

yy is the current value of the dependent variable vector, $y(t)$.

yp is the current value of $\dot{y}(t)$.

rr is the output residual vector $F(t, y, \dot{y})$.

user_data is a pointer to user data, the same as the user_data parameter passed to IDASetUserData.

Return value An IDAResFn function type should return a value of 0 if successful, a positive value if a recoverable error occurred (e.g. yy has an illegal value), or a negative value if a nonrecoverable error occurred. In the last case, the integrator halts. If a recoverable error occurred, the integrator will attempt to correct and retry.

Notes A recoverable failure error return from the IDAResFn is typically used to flag a value of the dependent variable y that is "illegal" in some way (e.g., negative where only a non-negative value is physically meaningful). If such a return is made, IDAS will attempt to recover (possibly repeating the Newton iteration, or reducing the step size) in order to avoid this recoverable error return.

For efficiency reasons, the DAE residual function is not evaluated at the converged solution of the nonlinear solver. Therefore, in general, a recoverable error in that converged value cannot be corrected. (It may be detected when the right-hand side function is called the first time during the following integration step, but a successful step cannot be undone.) However, if the user program also includes quadrature integration, the state variables can be checked for legality in the call to IDAQuadRhsFn, which is called at the converged solution of the nonlinear system, and therefore IDAS can be flagged to attempt to recover from such a situation. Also, if sensitivity analysis is performed with the staggered method, the DAE residual function is called at the converged solution of the nonlinear system, and a recoverable error at that point can be flagged, and IDAS will then try to correct it.

Allocation of memory for yp is handled within IDAS.

4.6.2 Error message handler function

As an alternative to the default behavior of directing error and warning messages to the file pointed to by errfp (see IDASetErrFile), the user may provide a function of type IDAErrHandlerFn to process any such messages. The function type IDAErrHandlerFn is defined as follows:

IDAErrHandlerFn

Definition
```
typedef void (*IDAErrHandlerFn)(int error_code, const char *module,
                                const char *function, char *msg,
                                void *eh_data);
```

Purpose This function processes error and warning messages from IDAS and its sub-modules.

Arguments
error_code is the error code.

module is the name of the IDAS module reporting the error.

function is the name of the function in which the error occurred.

msg is the error message.

eh_data is a pointer to user data, the same as the eh_data parameter passed to IDASetErrHandlerFn.

Return value A IDAErrHandlerFn function has no return value.

Notes error_code is negative for errors and positive (IDA_WARNING) for warnings. If a function that returns a pointer to memory encounters an error, it sets error_code to 0.

4.6.3 Error weight function

As an alternative to providing the relative and absolute tolerances, the user may provide a function of type `IDAEwtFn` to compute a vector `ewt` containing the multiplicative weights W_i used in the WRMS norm $\| v\|_{\text{WRMS}} = \sqrt{(1/N)\sum_1^N (W_i \cdot v_i)^2}$. These weights will used in place of those defined by Eq. (2.7). The function type `IDAEwtFn` is defined as follows:

`IDAEwtFn`

Definition `typedef int (*IDAEwtFn)(N_Vector y, N_Vector ewt, void *user_data);`

Purpose This function computes the WRMS error weights for the vector y.

Arguments
- `y` is the value of the dependent variable vector at which the weight vector is to be computed.
- `ewt` is the output vector containing the error weights.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDAEwtFn` function type must return 0 if it successfully set the error weights and -1 otherwise.

Notes Allocation of memory for `ewt` is handled within IDAS.

The error weight vector must have all components positive. It is the user's responsiblity to perform this test and return -1 if it is not satisfied.

4.6.4 Rootfinding function

If a rootfinding problem is to be solved during the integration of the DAE system, the user must supply a C function of type `IDARootFn`, defined as follows:

`IDARootFn`

Definition
```
typedef int (*IDARootFn)(realtype t, N_Vector y, N_Vector yp,
                         realtype *gout, void *user_data);
```

Purpose This function computes a vector-valued function $g(t, y, \dot{y})$ such that the roots of the `nrtfn` components $g_i(t, y, \dot{y})$ are to be found during the integration.

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, $y(t)$.
- `yp` is the current value of $\dot{y}(t)$, the $t-$derivative of y.
- `gout` is the output array, of length `nrtfn`, with components $g_i(t, y, \dot{y})$.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDARootFn` should return 0 if successful or a non-zero value if an error occurred (in which case the integration is halted and `IDASolve` returns `IDA_RTFUNC_FAIL`).

Notes Allocation of memory for `gout` is handled within IDAS.

4.6.5 Jacobian information (direct method with dense Jacobian)

If the direct linear solver with dense treatment of the Jacobian is used (i.e. either `IDADense` or `IDALapackDense` is called in Step 8 of §4.4), the user may provide a function of type `IDADlsDenseJacFn` defined by

IDADlsDenseJacFn

Definition
```
typedef int (*IDADlsDenseJacFn)(sunindextype Neq, realtype tt, realtype cj,
                                N_Vector yy, N_Vector yp, N_Vector rr,
                                DlsMat Jac, void *user_data,
                                N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the dense Jacobian J of the DAE system (or an approximation to it), defined by Eq. (2.6).

Arguments

Neq	is the problem size (number of equations).
tt	is the current value of the independent variable t.
cj	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
yy	is the current value of the dependent variable vector, $y(t)$.
yp	is the current value of $\dot{y}(t)$.
rr	is the current value of the residual vector $F(t, y, \dot{y})$.
Jac	is the output (approximate) Jacobian matrix, $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$.
user_data	is a pointer to user data, the same as the user_data parameter passed to IDASetUserData.
tmp1	
tmp2	
tmp3	are pointers to memory allocated for variables of type N_Vector which can be used by IDADlsDenseJacFn as temporary storage or work space.

Return value An IDADlsDenseJacFn function type should return 0 if successful, a positive value if a recoverable error occurred, or a negative value if a nonrecoverable error occurred.

In the case of a recoverable eror return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (2.6).

Notes A user-supplied dense Jacobian function must load the Neq $\times$ Neq dense matrix Jac with an approximation to the Jacobian matrix $J(t, y, \dot{y})$ at the point (tt, yy, yp). Only nonzero elements need to be loaded into Jac because Jac is set to the zero matrix before the call to the Jacobian function. The type of Jac is DlsMat (described below and in §11.1).

The accessor macros DENSE_ELEM and DENSE_COL allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the DlsMat type. DENSE_ELEM(Jac, i, j) references the (i, j)-th element of the dense matrix Jac (i, j= 0... Neq−1). This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to Neq, the Jacobian element $J_{m,n}$ can be loaded with the statement DENSE_ELEM(Jac, m-1, n-1) = $J_{m,n}$. Alternatively, DENSE_COL(Jac, j) returns a pointer to the storage for the jth column of Jac (j= 0... Neq−1), and the elements of the j-th column are then accessed via ordinary array indexing. Thus $J_{m,n}$ can be loaded with the statements col_n = DENSE_COL(Jac, n-1); col_n[m-1] = $J_{m,n}$. For large problems, it is more efficient to use DENSE_COL than to use DENSE_ELEM. Note that both of these macros number rows and columns starting from 0, not 1.

The DlsMat type and the accessor macros DENSE_ELEM and DENSE_COL are documented in §11.1.

If the user's IDADlsDenseJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to ida_mem to user_data and then use the IDAGet* functions described in §4.5.9.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

For the sake of uniformity, the argument `Neq` is of type `sunindextype`, even in the case that the Lapack dense solver is to be used.

4.6.6 Jacobian information (direct method with banded Jacobian)

If the direct linear solver with banded treatment of the Jacobian is used (i.e. either `IDABand` or `IDALapackBand` is called in Step 8 of §4.4), the user may provide a function of type `IDADlsBandJacFn` defined as follows:

`IDADlsBandJacFn`

Definition
```
typedef int (*IDADlsBandJacFn)(sunindextype Neq, sunindextype mupper,
                               sunindextype mlower, realtype tt, realtype cj,
                               N_Vector yy, N_Vector yp, N_Vector rr,
                               DlsMat Jac, void *user_data,
                               N_Vector tmp1, N_Vector tmp2,N_Vector tmp3);
```

Purpose This function computes the banded Jacobian J of the DAE system (or a banded approximation to it), defined by Eq. (2.6).

Arguments

`Neq`	is the problem size.
`mupper`	
`mlower`	are the upper and lower half bandwidth of the Jacobian.
`tt`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.
`yp`	is the current value of $\dot{y}(t)$.
`rr`	is the current value of the residual vector $F(t, y, \dot{y})$.
`cj`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`Jac`	is the output (approximate) Jacobian matrix, $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.
`tmp1`	
`tmp2`	
`tmp3`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADlsBandJacFn` as temporary storage or work space.

Return value A `IDADlsBandJacFn` function type should return 0 if successful, a positive value if a recoverable error occurred, or a negative value if a nonrecoverable error occurred.

In the case of a recoverable eror return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (2.6).

Notes A user-supplied band Jacobian function must load the band matrix `Jac` of type `DlsMat` with the elements of the Jacobian $J(t, y, \dot{y})$ at the point (`tt`, `yy`, `yp`). Only nonzero elements need to be loaded into `Jac` because `Jac` is preset to zero before the call to the Jacobian function.

The accessor macros `BAND_ELEM`, `BAND_COL`, and `BAND_COL_ELEM` allow the user to read and write band matrix elements without making specific references to the underlying representation of the `DlsMat` type. `BAND_ELEM(Jac, i, j)` references the (`i`, `j`)th element of the band matrix `Jac`, counting from 0. This macro is for use in small problems in which efficiency of access is not a major concern. Thus, in terms of indices m and n running from 1 to `Neq` with (m, n) within the band defined by `mupper` and `mlower`, the Jacobian element $J_{m,n}$ can be loaded with the statement `BAND_ELEM(Jac, m-1, n-1) =` $J_{m,n}$. The elements within the band are those with `-mupper` $\leq$ `m-n` $\leq$ `mlower`. Alternatively, `BAND_COL(Jac, j)` returns a pointer to the diagonal element of the `j`th

column of Jac, and if we assign this address to realtype *col_j, then the ith element of the jth column is given by BAND_COL_ELEM(col_j, i, j), counting from 0. Thus for (m, n) within the band, $J_{m,n}$ can be loaded by setting col_n = BAND_COL(Jac, n-1); BAND_COL_ELEM(col_n, m-1, n-1) = $J_{m,n}$. The elements of the jth column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type DlsMat. The array col_n can be indexed from −mupper to mlower. For large problems, it is more efficient to use the combination of BAND_COL and BAND_COL_ELEM than to use the BAND_ELEM. As in the dense case, these macros all number rows and columns starting from 0, not 1.

The DlsMat type and the accessor macros BAND_ELEM, BAND_COL, and BAND_COL_ELEM are documented in §11.1.

If the user's IDADlsBandJacFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to ida_mem to user_data and then use the IDAGet* functions described in §4.5.9.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

For the sake of uniformity, the arguments Neq, mlower, and mupper are of type sunindextype, even in the case that the Lapack band solver is to be used.

4.6.7 Jacobian information (direct method with sparse Jacobian)

If the direct linear solver with sparse treatment of the Jacobian is used (i.e. either IDAKLU or IDASuperLUMT is called in Step 8 of §4.4), the user must provide a function of type IDASlsSparseJacFn defined as follows:

IDASlsSparseJacFn

Definition
```
typedef int (*IDASlsSparseJacFn)(realtype t, realtype c_j,
                                 N_Vector y, N_Vector yp, N_Vector r,
                                 SlsMat Jac, void *user_data,
                                 N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the sparse Jacobian J of the DAE system (or an approximation to it), defined by Eq. (2.6).

Arguments

t	is the current value of the independent variable.
y	is the current value of the dependent variable vector, $y(t)$.
yp	is the current value of $\dot{y}(t)$.
r	is the current value of the residual vector $F(t, y, \dot{y})$.
c_j	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
Jac	is the output (approximate) Jacobian matrix, $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$.
user_data	is a pointer to user data, the same as the user_data parameter passed to IDASetUserData.
tmp1	
tmp2	
tmp3	are pointers to memory allocated for variables of type N_Vector which can be used by IDASlsSparseJacFn as temporary storage or work space.

Return value A IDASlsSparseJacFn function type should return 0 if successful, a positive value if a recoverable error occurred, or a negative value if a nonrecoverable error occurred.

In the case of a recoverable error return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (2.6).

Notes A user-supplied sparse Jacobian function must load the compressed-sparse-column matrix `Jac` with the elements of the Jacobian $J(t, y, \dot{y})$ at the point (`t`, `y`, `yp`). Storage for `Jac` already exists on entry to this function, although the user should ensure that sufficient space is allocated in `Jac` to hold the nonzero values to be set; if the existing space is insufficient the user may reallocate the data and row index arrays as needed. The type of `Jac` is `SlsMat`, and the amount of allocated space is available within the `SlsMat` structure as `NNZ`. The `SlsMat` type is further documented in the Section §11.2.

If the user's `IDASlsSparseJacFn` function uses difference quotient approximations to set the specific nonzero matrix entries, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `ida_mem` to `user_data` and then use the `IDAGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

4.6.8 Jacobian information (matrix-vector product)

If one of the Krylov iterative linear solvers SPGMR, SPBCGS, or SPTFQMR is selected (`IDASp*` is called in step 8 of §4.4), the user may provide a function of type `IDASpilsJacTimesVecFn`, described below, to compute matrix-vector products Jv. If such a function is not supplied, the default is a difference quotient approximation to these products.

`IDASpilsJacTimesVecFn`

Definition
```
typedef int (*IDASpilsJacTimesVecFn)(realtype tt, N_Vector yy,
                                     N_Vector yp, N_Vector rr,
                                     N_Vector v, N_Vector Jv,
                                     realtype cj, void *user_data,
                                     N_Vector tmp1, N_Vector tmp2);
```

Purpose This function computes the product Jv of the DAE system Jacobian J (or an approximation to it) and a given vector `v`, where J is defined by Eq. (2.6).

Arguments

`tt`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.
`yp`	is the current value of $\dot{y}(t)$.
`rr`	is the current value of the residual vector $F(t, y, \dot{y})$.
`v`	is the vector by which the Jacobian must be multiplied to the right.
`Jv`	is the computed output vector.
`cj`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.
`tmp1`	
`tmp2`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDASpilsJacTimesVecFn` as temporary storage or work space.

Return value The value to be returned by the Jacobian-times-vector function should be 0 if successful. A nonzero value indicates that a nonrecoverable error occurred.

Notes If the user's `IDASpilsJacTimesVecFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to `ida_mem` to `user_data` and then use the `IDAGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

4.6.9 Preconditioning (linear system solution)

If preconditioning is used, then the user must provide a C function to solve the linear system $Pz = r$ where P is a left preconditioner matrix which approximates (at least crudely) the Jacobian matrix $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$. This function must be of type `IDASpilsPrecSolveFn`, defined as follows:

`IDASpilsPrecSolveFn`

Definition
```
typedef int (*IDASpilsPrecSolveFn)(realtype tt, N_Vector yy,
                                   N_Vector yp, N_Vector rr,
                                   N_Vector rvec, N_Vector zvec,
                                   realtype cj, realtype delta,
                                   void *user_data, N_Vector tmp);
```

Purpose This function solves the preconditioning system $Pz = r$.

Arguments

`tt`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.
`yp`	is the current value of $\dot{y}(t)$.
`rr`	is the current value of the residual vector $F(t, y, \dot{y})$.
`rvec`	is the right-hand side vector r of the linear system to be solved.
`zvec`	is the computed output vector.
`cj`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`delta`	is an input tolerance to be used if an iterative method is employed in the solution. In that case, the residual vector $Res = r - Pz$ of the system should be made less than `delta` in weighted l_2 norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} <$ `delta`. To obtain the `N_Vector ewt`, call `IDAGetErrWeights` (see §4.5.9.2).
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to the function `IDASetUserData`.
`tmp`	is a pointer to memory allocated for a variable of type `N_Vector` which can be used for work space.

Return value The value to be returned by the preconditioner solve function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), negative for an unrecoverable error (in which case the integration is halted).

4.6.10 Preconditioning (Jacobian data)

If the user's preconditioner requires that any Jacobian-related data be evaluated or preprocessed, then this needs to be done in a user-supplied C function of type `IDASpilsPrecSetupFn`, defined as follows:

`IDASpilsPrecSetupFn`

Definition
```
typedef int (*IDASpilsPrecSetupFn)(realtype tt, N_Vector yy,
                                   N_Vector yp, N_Vector rr,
                                   realtype cj, void *user_data,
                                   N_Vector tmp1, N_Vector tmp2,
                                   N_Vector tmp3);
```

Purpose This function evaluates and/or preprocesses Jacobian-related data needed by the preconditioner.

Arguments The arguments of an `IDASpilsPrecSetupFn` are as follows:

`tt`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.

`yp`	is the current value of $\dot{y}(t)$.
`rr`	is the current value of the residual vector $F(t, y, \dot{y})$.
`cj`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to the function `IDASetUserData`.
`tmp1`	
`tmp2`	
`tmp3`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDASpilsPrecSetupFn` as temporary storage or work space.

Return value The value to be returned by the preconditioner setup function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), negative for an unrecoverable error (in which case the integration is halted).

Notes The operations performed by this function might include forming a crude approximate Jacobian, and performing an LU factorization on the resulting approximation.

Each call to the preconditioner setup function is preceded by a call to the `IDAResFn` user function with the same (`tt`, `yy`, `yp`) arguments. Thus the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual.

This function is not called in advance of every call to the preconditioner solve function, but rather is called only as often as needed to achieve convergence in the Newton iteration.

If the user's `IDASpilsPrecSetupFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to `ida_mem` to `user_data` and then use the `IDAGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

4.7 Integration of pure quadrature equations

IDAS allows the DAE system to include *pure quadratures*. In this case, it is more efficient to treat the quadratures separately by excluding them from the nonlinear solution stage. To do this, begin by excluding the quadrature variables from the vectors `yy` and `yp` and the quadrature equations from within `res`. Thus a separate vector `yQ` of quadrature variables is to satisfy $(d/dt)\texttt{yQ} = f_Q(t, y, \dot{y})$. The following is an overview of the sequence of calls in a user's main program in this situation. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. **Initialize parallel or multi-threaded environment, if appropriate**
2. **Set problem dimensions, etc.**

   This generally includes `N`, the problem size N (excluding quadrature variables), `Nq`, the number of quadrature variables, and may include the local vector length `Nlocal` (excluding quadrature variables), and local number of quadrature variables `Nqlocal`.
3. **Set vectors of initial values**
4. **Create IDAS object**
5. **Allocate internal memory**
6. **Set optional inputs**

7. **Attach linear solver module**

8. **Set linear solver optional inputs**

9. **Set vector of initial values for quadrature variables**

   Typically, the quadrature variables should be initialized to 0.

10. **Initialize quadrature integration**

    Call `IDAQuadInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §4.7.1 for details.

11. **Set optional inputs for quadrature integration**

    Call `IDASetQuadErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `IDAQuad*tolerances` functions must be called to specify the integration tolerances for quadrature variables. See §4.7.4 for details.

12. **Advance solution in time**

13. **Extract quadrature variables**

    Call `IDAGetQuad` or `IDAGetQuadDky` to obtain the values of the quadrature variables or their derivatives at the current time. See §4.7.3 for details.

14. **Get optional outputs**

15. **Get quadrature optional outputs**

    Call `IDAGetQuad*` functions to obtain optional output related to the integration of quadratures. See §4.7.5 for details.

16. **Deallocate memory for solution vectors and for the vector of quadrature variables**

17. **Free solver memory**

18. **Finalize MPI, if used**

`IDAQuadInit` can be called and quadrature-related optional inputs (step 11 above) can be set, anywhere between steps 4 and 12.

4.7.1 Quadrature initialization and deallocation functions

The function `IDAQuadInit` activates integration of quadrature equations and allocates internal memory related to these calculations. The form of the call to this function is as follows:

`IDAQuadInit`

Call `flag = IDAQuadInit(ida_mem, rhsQ, yQ0);`

Description The function `IDAQuadInit` provides required problem specifications, allocates internal memory, and initializes quadrature integration.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `rhsQ` (`IDAQuadRhsFn`) is the C function which computes f_Q, the right-hand side of the quadrature equations. This function has the form `fQ(t, yy, yp, rhsQ, user_data)` (for full details see §4.7.6).
- `yQ0` (`N_Vector`) is the initial value of y_Q.

Return value The return value `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAQuadInit` was successful.

`IDA_MEM_NULL` The IDAS memory was not initialized by a prior call to `IDACreate`.

`IDA_MEM_FAIL` A memory allocation request failed.

Notes If an error occurred, `IDAQuadInit` also sends an error message to the error handler function.

In terms of the number of quadrature variables N_q and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value: `lenrw` = `lenrw` + (`maxord`+5)N_q
- If `IDAQuadSVtolerances` is called: `lenrw` = `lenrw` +N_q

and the size of the integer workspace is increased as follows:

- Base value: `leniw` = `leniw` + (`maxord`+5)N_q
- If `IDAQuadSVtolerances` is called: `leniw` = `leniw` +N_q

The function `IDAQuadReInit`, useful during the solution of a sequence of problems of same size, reinitializes the quadrature-related internal memory and must follow a call to `IDAQuadInit` (and maybe a call to `IDAReInit`). The number `Nq` of quadratures is assumed to be unchanged from the prior call to `IDAQuadInit`. The call to the `IDAQuadReInit` function has the following form:

`IDAQuadReInit`

Call `flag = IDAQuadReInit(ida_mem, yQ0);`

Description The function `IDAQuadReInit` provides required problem specifications and reinitializes the quadrature integration.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`yQ0` (`N_Vector`) is the initial value of y_Q.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS` The call to `IDAReInit` was successful.

`IDA_MEM_NULL` The IDAS memory was not initialized by a prior call to `IDACreate`.

`IDA_NO_QUAD` Memory space for the quadrature integration was not allocated by a prior call to `IDAQuadInit`.

Notes If an error occurred, `IDAQuadReInit` also sends an error message to the error handler function.

`IDAQuadFree`

Call `IDAQuadFree(ida_mem);`

Description The function `IDAQuadFree` frees the memory allocated for quadrature integration.

Arguments The argument is the pointer to the IDAS memory block (of type `void *`).

Return value The function `IDAQuadFree` has no return value.

Notes In general, `IDAQuadFree` need not be called by the user as it is invoked automatically by `IDAFree`.

4.7.2 IDAS solver function

Even if quadrature integration was enabled, the call to the main solver function `IDASolve` is exactly the same as in §4.5.6. However, in this case the return value `flag` can also be one of the following:

`IDA_QRHS_FAIL` The quadrature right-hand side function failed in an unrecoverable manner.

`IDA_FIRST_QRHS_ERR` The quadrature right-hand side function failed at the first call.

IDA_REP_QRHS_ERR	Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. This value will also be returned if the quadrature right-hand side function had repeated recoverable errors during the estimation of an initial step size (assuming the quadrature variables are included in the error tests).

4.7.3 Quadrature extraction functions

If quadrature integration has been initialized by a call to IDAQuadInit, or reinitialized by a call to IDAQuadReInit, then IDAS computes both a solution and quadratures at time t. However, IDASolve will still return only the solution y in y. Solution quadratures can be obtained using the following function:

IDAGetQuad

Call `flag = IDAGetQuad(ida_mem, &tret, yQ);`

Description The function IDAGetQuad returns the quadrature solution vector after a successful return from IDASolve.

Arguments

ida_mem	(void *) pointer to the memory previously allocated by IDAInit.
tret	(realtype) the time reached by the solver (output).
yQ	(N_Vector) the computed quadrature vector.

Return value The return value flag of IDAGetQuad is one of:

IDA_SUCCESS	IDAGetQuad was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_QUAD	Quadrature integration was not initialized.
IDA_BAD_DKY	yQ is NULL.

The function IDAGetQuadDky computes the k-th derivatives of the interpolating polynomials for the quadrature variables at time t. This function is called by IDAGetQuad with k = 0 and with the current time at which IDASolve has returned, but may also be called directly by the user.

IDAGetQuadDky

Call `flag = IDAGetQuadDky(ida_mem, t, k, dkyQ);`

Description The function IDAGetQuadDky returns derivatives of the quadrature solution vector after a successful return from IDASolve.

Arguments

ida_mem	(void *) pointer to the memory previously allocated by IDAInit.
t	(realtype) the time at which quadrature information is requested. The time t must fall within the interval defined by the last successful step taken by IDAS.
k	(int) order of the requested derivative. This must be $\leq klast$.
dkyQ	(N_Vector) the vector containing the derivative. This vector must be allocated by the user.

Return value The return value flag of IDAGetQuadDky is one of:

IDA_SUCCESS	IDAGetQuadDky succeeded.
IDA_MEM_NULL	The pointer to ida_mem was NULL.
IDA_NO_QUAD	Quadrature integration was not initialized.
IDA_BAD_DKY	The vector dkyQ is NULL.
IDA_BAD_K	k is not in the range $0, 1, ..., klast$.
IDA_BAD_T	The time t is not in the allowed range.

4.7.4 Optional inputs for quadrature integration

IDAS provides the following optional input functions to control the integration of quadrature equations.

`IDASetQuadErrCon`

Call `flag = IDASetQuadErrCon(ida_mem, errconQ);`

Description The function `IDASetQuadErrCon` specifies whether or not the quadrature variables are to be used in the step size control mechanism within IDAS. If they are, the user must call either `IDAQuadSStolerances` or `IDAQuadSVtolerances` to specify the integration tolerances for the quadrature variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`errconQ` (`booleantype`) specifies whether quadrature variables are included (`TRUE`) or not (`FALSE`) in the error control mechanism.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`
`IDA_NO_QUAD`	Quadrature integration has not been initialized.

Notes By default, `errconQ` is set to `FALSE`.
It is illegal to call `IDASetQuadErrCon` before a call to `IDAQuadInit`.

If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

`IDAQuadSStolerances`

Call `flag = IDAQuadSVtolerances(ida_mem, reltolQ, abstolQ);`

Description The function `IDAQuadSStolerances` specifies scalar relative and absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`reltolQ` (`realtype`) is the scalar relative error tolerance.
`abstolQ` (`realtype`) is the scalar absolute error tolerance.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_NO_QUAD`	Quadrature integration was not initialized.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

`IDAQuadSVtolerances`

Call `flag = IDAQuadSVtolerances(ida_mem, reltolQ, abstolQ);`

Description The function `IDAQuadSVtolerances` specifies scalar relative and vector absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`reltolQ` (`realtype`) is the scalar relative error tolerance.
`abstolQ` (`N_Vector`) is the vector absolute error tolerance.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_NO_QUAD`	Quadrature integration was not initialized.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

4.7.5 Optional outputs for quadrature integration

IDAS provides the following functions that can be used to obtain solver performance information related to quadrature integration.

`IDAGetQuadNumRhsEvals`

Call `flag = IDAGetQuadNumRhsEvals(ida_mem, &nrhsQevals);`

Description The function `IDAGetQuadNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`nrhsQevals` (`long int`) number of calls made to the user's `rhsQ` function.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional output value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_NO_QUAD` Quadrature integration has not been initialized.

`IDAGetQuadNumErrTestFails`

Call `flag = IDAGetQuadNumErrTestFails(ida_mem, &nQetfails);`

Description The function `IDAGetQuadNumErrTestFails` returns the number of local error test failures due to quadrature variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`nQetfails` (`long int`) number of error test failures due to quadrature variables.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional output value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_NO_QUAD` Quadrature integration has not been initialized.

`IDAGetQuadErrWeights`

Call `flag = IDAGetQuadErrWeights(ida_mem, eQweight);`

Description The function `IDAGetQuadErrWeights` returns the quadrature error weights at the current time.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`eQweight` (`N_Vector`) quadrature error weights at the current time.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional output value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_NO_QUAD` Quadrature integration has not been initialized.

Notes The user must allocate memory for `eQweight`.

If quadratures were not included in the error control mechanism (through a call to `IDASetQuadErrCon` with `errconQ = TRUE`), `IDAGetQuadErrWeights` does not set the `eQweight` vector.

IDAGetQuadStats

Call `flag = IDAGetQuadStats(ida_mem, &nrhsQevals, &nQetfails);`

Description The function `IDAGetQuadStats` returns the IDAS integrator statistics as a group.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nrhsQevals` (`long int`) number of calls to the user's `rhsQ` function.
`nQetfails` (`long int`) number of error test failures due to quadrature variables.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	the optional output values have been successfully set.
`IDA_MEM_NULL`	the `ida_mem` pointer is `NULL`.
`IDA_NO_QUAD`	Quadrature integration has not been initialized.

4.7.6 User-supplied function for quadrature integration

For integration of quadrature equations, the user must provide a function that defines the right-hand side of the quadrature equations (in other words, the integrand function of the integral that must be evaluated). This function must be of type `IDAQuadRhsFn` defined as follows:

IDAQuadRhsFn

Definition
```
typedef int (*IDAQuadRhsFn)(realtype t, N_Vector yy, N_Vector yp,
                            N_Vector rhsQ, void *user_data);
```

Purpose This function computes the quadrature equation right-hand side for a given value of the independent variable t and state vectors y and $\dot{y}$.

Arguments

`t`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.
`yp`	is the current value of the dependent variable derivative vector, $\dot{y}(t)$.
`rhsQ`	is the output vector $f_Q(t, y, \dot{y})$.
`user_data`	is the `user_data` pointer passed to `IDASetUserData`.

Return value A `IDAQuadRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDA_QRHS_FAIL` is returned).

Notes Allocation of memory for `rhsQ` is automatically handled within IDAS.

Both `y` and `rhsQ` are of type `N_Vector`, but they typically have different internal representations. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

There is one situation in which recovery is not possible even if `IDAQuadRhsFn` function returns a recoverable error flag. This is when this occurs at the very first call to the `IDAQuadRhsFn` (in which case IDAS returns `IDA_FIRST_QRHS_ERR`).

4.8 A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel DAE solver such as IDAS lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (2.5) that must be solved at each time step. The linear algebraic system is large, sparse, and structured. However, if a Krylov iterative method is to be effective in this setting, then a nontrivial preconditioner needs to be

used. Otherwise, the rate of convergence of the Krylov iterative method is usually unacceptably slow. Unfortunately, an effective preconditioner tends to be problem-specific.

However, we have developed one type of preconditioner that treats a rather broad class of PDE-based problems. It has been successfully used for several realistic, large-scale problems [26] and is included in a software module within the IDAS package. This module works with the parallel vector module NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix. The blocks need not have the same number of super- and sub-diagonals and these numbers may vary from block to block. This Band-Block-Diagonal Preconditioner module is called IDABBDPRE.

One way to envision these preconditioners is to think of the domain of the computational PDE problem as being subdivided into M non-overlapping sub-domains. Each of these sub-domains is then assigned to one of the M processors to be used to solve the DAE system. The basic idea is to isolate the preconditioning so that it is local to each processor, and also to use a (possibly cheaper) approximate residual function. This requires the definition of a new function $G(t, y, \dot{y})$ which approximates the function $F(t, y, \dot{y})$ in the definition of the DAE system (2.1). However, the user may set $G = F$. Corresponding to the domain decomposition, there is a decomposition of the solution vectors y and $\dot{y}$ into M disjoint blocks y_m and $\dot{y}_m$, and a decomposition of G into blocks G_m. The block G_m depends on y_m and $\dot{y}_m$, and also on components of $y_{m'}$ and $\dot{y}_{m'}$ associated with neighboring sub-domains (so-called ghost-cell data). Let $\bar{y}_m$ and $\bar{\dot{y}}_m$ denote y_m and $\dot{y}_m$ (respectively) augmented with those other components on which G_m depends. Then we have

$$G(t, y, \dot{y}) = [G_1(t, \bar{y}_1, \bar{\dot{y}}_1), G_2(t, \bar{y}_2, \bar{\dot{y}}_2), \ldots, G_M(t, \bar{y}_M, \bar{\dot{y}}_M)]^T \ , \tag{4.1}$$

and each of the blocks $G_m(t, \bar{y}_m, \bar{\dot{y}}_m)$ is uncoupled from the others.

The preconditioner associated with this decomposition has the form

$$P = diag[P_1, P_2, \ldots, P_M] \tag{4.2}$$

where

$$P_m \approx \partial G_m / \partial y_m + \alpha \partial G_m / \partial \dot{y}_m \tag{4.3}$$

This matrix is taken to be banded, with upper and lower half-bandwidths `mudq` and `mldq` defined as the number of non-zero diagonals above and below the main diagonal, respectively. The difference quotient approximation is computed using `mudq` + `mldq` +2 evaluations of G_m, but only a matrix of bandwidth `mukeep` + `mlkeep` +1 is retained.

Neither pair of parameters need be the true half-bandwidths of the Jacobians of the local block of G, if smaller values provide a more efficient preconditioner. Such an efficiency gain may occur if the couplings in the DAE system outside a certain bandwidth are considerably weaker than those within the band. Reducing `mukeep` and `mlkeep` while keeping `mudq` and `mldq` at their true values, discards the elements outside the narrower band. Reducing both pairs has the additional effect of lumping the outer Jacobian elements into the computed elements within the band, and requires more caution and experimentation.

The solution of the complete linear system

$$Px = b \tag{4.4}$$

reduces to solving each of the equations

$$P_m x_m = b_m \tag{4.5}$$

and this is done by banded LU factorization of P_m followed by a banded backsolve.

Similar block-diagonal preconditioners could be considered with different treatment of the blocks P_m. For example, incomplete LU factorization or an iterative method could be used instead of banded LU factorization.

The IDABBDPRE module calls two user-provided functions to construct P: a required function `Gres` (of type `IDABBDLocalFn`) which approximates the residual function $G(t, y, \dot{y}) \approx F(t, y, \dot{y})$ and which is computed locally, and an optional function `Gcomm` (of type `IDABBDCommFn`) which performs

all inter-process communication necessary to evaluate the approximate residual G. These are in addition to the user-supplied residual function `res`. Both functions take as input the same pointer `user_data` as passed by the user to `IDASetUserData` and passed to the user's function `res`. The user is responsible for providing space (presumably within `user_data`) for components of `yy` and `yp` that are communicated by `Gcomm` from the other processors, and that are then used by `Gres`, which should not do any communication.

`IDABBDLocalFn`

Definition
```
typedef int (*IDABBDLocalFn)(sunindextype Nlocal, realtype tt,
                             N_Vector yy, N_Vector yp, N_Vector gval,
                             void *user_data);
```

Purpose This `Gres` function computes $G(t, y, \dot{y})$. It loads the vector `gval` as a function of `tt`, `yy`, and `yp`.

Arguments
- `Nlocal` is the local vector length.
- `tt` is the value of the independent variable.
- `yy` is the dependent variable.
- `yp` is the derivative of the dependent variable.
- `gval` is the output vector.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDABBDLocalFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes This function must assume that all inter-processor communication of data needed to calculate `gval` has already been done, and this data is accessible within `user_data`.

The case where G is mathematically identical to F is allowed.

`IDABBDCommFn`

Definition
```
typedef int (*IDABBDCommFn)(sunindextype Nlocal, realtype tt,
                            N_Vector yy, N_Vector yp, void *user_data);
```

Purpose This `Gcomm` function performs all inter-processor communications necessary for the execution of the `Gres` function above, using the input vectors `yy` and `yp`.

Arguments
- `Nlocal` is the local vector length.
- `tt` is the value of the independent variable.
- `yy` is the dependent variable.
- `yp` is the derivative of the dependent variable.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDABBDCommFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes The `Gcomm` function is expected to save communicated data in space defined within the structure `user_data`.

Each call to the `Gcomm` function is preceded by a call to the residual function `res` with the same (`tt`, `yy`, `yp`) arguments. Thus `Gcomm` can omit any communications done by `res` if relevant to the evaluation of `Gres`. If all necessary communication was done in `res`, then `Gcomm` = `NULL` can be passed in the call to `IDABBDPrecInit` (see below).

Besides the header files required for the integration of the DAE problem (see §4.3), to use the IDABBDPRE module, the main program must include the header file `idas_bbdpre.h` which declares the needed function prototypes.

The following is a summary of the usage of this module and describes the sequence of calls in the user main program. Steps that are unchanged from the user main program presented in §4.4 are grayed-out.

1. **Initialize MPI**
2. **Set problem dimensions**
3. **Set vector of initial values**
4. **Create IDAS object**
5. **Allocate internal memory**
6. **Set optional inputs**
7. **Attach iterative linear solver, one of:**
   (a) `flag = IDASpgmr(ida_mem, maxl);`
   (b) `flag = IDASpbcg(ida_mem, maxl);`
   (c) `flag = IDASptfqmr(ida_mem, maxl);`
8. **Initialize the IDABBDPRE preconditioner module**
   Specify the upper and lower bandwidths `mudq`, `mldq` and `mukeep`, `mlkeep` and call
   ```
   flag = IDABBDPrecInit(ida_mem, Nlocal, mudq, mldq,
                         mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);
   ```
   to allocate memory and initialize the internal preconditioner data. The last two arguments of `IDABBDPrecInit` are the two user-supplied functions described above.
9. **Set linear solver optional inputs**
   Note that the user should not overwrite the preconditioner setup function or solve function through calls to IDASPILS optional input functions.
10. **Correct initial values**
11. **Specify rootfinding problem**
12. **Advance solution in time**
13. **Get optional outputs**
    Additional optional outputs associated with IDABBDPRE are available by way of two routines described below, `IDABBDPrecGetWorkSpace` and `IDABBDPrecGetNumGfnEvals`.
14. **Deallocate memory for solution vector**
15. **Free solver memory**
16. **Finalize MPI**

The user-callable functions that initialize (step 8 above) or re-initialize the IDABBDPRE preconditioner module are described next.

`IDABBDPrecInit`

Call `flag = IDABBDPrecInit(ida_mem, Nlocal, mudq, mldq, mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);`

Description The function `IDABBDPrecInit` initializes and allocates (internal) memory for the IDABBDPRE preconditioner.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `Nlocal` (`sunindextype`) local vector dimension.
- `mudq` (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mldq` (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mukeep` (`sunindextype`) upper half-bandwidth of the retained banded approximate Jacobian block.
- `mlkeep` (`sunindextype`) lower half-bandwidth of the retained banded approximate Jacobian block.
- `dq_rel_yy` (`realtype`) the relative increment in components of `y` used in the difference quotient approximations. The default is `dq_rel_yy`$= \sqrt{\text{unit roundoff}}$, which can be specified by passing `dq_rel_yy`$= 0.0$.
- `Gres` (`IDABBDLocalFn`) the C function which computes the local residual approximation $G(t, y, \dot{y})$.
- `Gcomm` (`IDABBDCommFn`) the optional C function which performs all inter-process communication required for the computation of $G(t, y, \dot{y})$.

Return value The return value `flag` (of type `int`) is one of
- `IDASPILS_SUCCESS` The call to `IDABBDPrecInit` was successful.
- `IDASPILS_MEM_NULL` The `ida_mem` pointer was `NULL`.
- `IDASPILS_MEM_FAIL` A memory allocation request has failed.
- `IDASPILS_LMEM_NULL` An IDASPILS linear solver memory was not attached.
- `IDASPILS_ILL_INPUT` The supplied vector implementation was not compatible with block band preconditioner.

Notes If one of the half-bandwidths `mudq` or `mldq` to be used in the difference-quotient calculation of the approximate Jacobian is negative or exceeds the value `Nlocal`-1, it is replaced by 0 or `Nlocal`-1 accordingly.

The half-bandwidths `mudq` and `mldq` need not be the true half-bandwidths of the Jacobian of the local block of G, when smaller values may provide a greater efficiency.

Also, the half-bandwidths `mukeep` and `mlkeep` of the retained banded approximate Jacobian block may be even smaller, to reduce storage and computation costs further.

For all four half-bandwidths, the values need not be the same on every processor.

The IDABBDPRE module also provides a reinitialization function to allow for a sequence of problems of the same size with IDASPGMR/IDABBDPRE, IDASPBCG/IDABBDPRE, or IDASPTFQMR/IDABBDPRE, provided there is no change in `local_N`, `mukeep`, or `mlkeep`. After solving one problem, and after calling `IDAReInit` to re-initialize IDAS for a subsequent problem, a call to `IDABBDPrecReInit` can be made to change any of the following: the half-bandwidths `mudq` and `mldq` used in the difference-quotient Jacobian approximations, the relative increment `dq_rel_yy`, or one of the user-supplied functions `Gres` and `Gcomm`.

`IDABBDPrecReInit`

Call `flag = IDABBDPrecReInit(ida_mem, mudq, mldq, dq_rel_yy);`

Description The function `IDABBDPrecReInit` reinitializes the IDABBDPRE preconditioner.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `mudq` (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.

`mldq` (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.

`dq_rel_yy` (`realtype`) the relative increment in components of `y` used in the difference quotient approximations. The default is `dq_rel_yy` $= \sqrt{\text{unit roundoff}}$, which can be specified by passing `dq_rel_yy` $= 0.0$.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The call to `IDABBDPrecReInit` was successful.

`IDASPILS_MEM_NULL` The `ida_mem` pointer was `NULL`.

`IDASPILS_LMEM_NULL` An IDASPILS linear solver memory was not attached.

`IDASPILS_PMEM_NULL` The function `IDABBDPrecInit` was not previously called.

Notes If one of the half-bandwidths `mudq` or `mldq` is negative or exceeds the value `Nlocal`-1, it is replaced by 0 or `Nlocal`-1, accordingly.

The following two optional output functions are available for use with the IDABBDPRE module:

`IDABBDPrecGetWorkSpace`

Call `flag = IDABBDPrecGetWorkSpace(ida_mem, &lenrwBBDP, &leniwBBDP);`

Description The function `IDABBDPrecGetWorkSpace` returns the local sizes of the IDABBDPRE real and integer workspaces.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`lenrwBBDP` (`long int`) local number of real values in the IDABBDPRE workspace.

`leniwBBDP` (`long int`) local number of integer values in the IDABBDPRE workspace.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional output value has been successfully set.

`IDASPILS_MEM_NULL` The `ida_mem` pointer was `NULL`.

`IDASPILS_PMEM_NULL` The IDABBDPRE preconditioner has not been initialized.

Notes In terms of the local vector dimension N_l, and `smu` $= \min(N_l - 1,$ `mukeep` $+$ `mlkeep`$)$, the actual size of the real workspace is N_l (2 `mlkeep` $+$ `mukeep` $+$ `smu` $+2$) `realtype` words. The actual size of the integer workspace is N_l integer words.

`IDABBDPrecGetNumGfnEvals`

Call `flag = IDABBDPrecGetNumGfnEvals(ida_mem, &ngevalsBBDP);`

Description The function `IDABBDPrecGetNumGfnEvals` returns the cumulative number of calls to the user `Gres` function due to the finite difference approximation of the Jacobian blocks used within IDABBDPRE's preconditioner setup function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`ngevalsBBDP` (`long int`) the cumulative number of calls to the user `Gres` function.

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS` The optional output value has been successfully set.

`IDASPILS_MEM_NULL` The `ida_mem` pointer was `NULL`.

`IDASPILS_PMEM_NULL` The IDABBDPRE preconditioner has not been initialized.

In addition to the `ngevalsBBDP` `Gres` evaluations, the costs associated with IDABBDPRE also include `nlinsetups` LU factorizations, `nlinsetups` calls to `Gcomm`, `npsolves` banded backsolve calls, and `nrevalsLS` residual function evaluations, where `nlinsetups` is an optional IDAS output (see §4.5.9.2), and `npsolves` and `nrevalsLS` are linear solver optional outputs (see §4.5.9.7).

Chapter 5

Using IDAS for Forward Sensitivity Analysis

This chapter describes the use of IDAS to compute solution sensitivities using forward sensitivity analysis. One of our main guiding principles was to design the IDAS user interface for forward sensitivity analysis as an extension of that for IVP integration. Assuming a user main program and user-defined support routines for IVP integration have already been defined, in order to perform forward sensitivity analysis the user only has to insert a few more calls into the main program and (optionally) define an additional routine which computes the residuals for sensitivity systems (2.12). The only departure from this philosophy is due to the `IDAResFn` type definition (§4.6.1). Without changing the definition of this type, the only way to pass values of the problem parameters to the DAE residual function is to require the user data structure `user_data` to contain a pointer to the array of real parameters p.

IDAS uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in Appendix B.

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable routines and of the user-supplied routines that were not already described in Chapter 4.

5.1 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) as an application of IDAS. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the NVECTOR implementation used. For the steps that are not, refer to Chapter 7 for the specific names. Differences between the user main program in §4.4 and the one below start only at step (11). Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

First, note that no additional header files need be included for forward sensitivity analysis beyond those for IVP solution (§4.4).

1. **Initialize parallel or multi-threaded environment**
2. **Set problem dimensions etc.**
3. **Set initial values**
4. **Create IDAS object**
5. **Allocate internal memory**
6. **Specify integration tolerances**

7. **Set optional inputs**
8. **Attach linear solver module**
9. **Set linear solver optional inputs**
10. **Initialize quadrature problem, if not sensitivity-dependent**
11. **Define the sensitivity problem**

    •Number of sensitivities (required)
    Set `Ns` $= N_s$, the number of parameters with respect to which sensitivities are to be computed.

    •Problem parameters (optional)
    If IDAS is to evaluate the residuals of the sensitivity systems, set `p`, an array of `Np` real parameters upon which the IVP depends. Only parameters with respect to which sensitivities are (potentially) desired need to be included. Attach `p` to the user data structure `user_data`. For example, `user_data->p = p;`
    If the user provides a function to evaluate the sensitivity residuals, `p` need not be specified.

    •Parameter list (optional)
    If IDAS is to evaluate the sensitivity residuals, set `plist`, an array of `Ns` integers to specify the parameters `p` with respect to which solution sensitivities are to be computed. If sensitivities with respect to the j-th parameter `p[j]` ($0 \le$ `j` $<$ `Np`) are desired, set $\text{plist}_i = j$, for some $i = 0, \ldots, N_s - 1$.
    If `plist` is not specified, IDAS will compute sensitivities with respect to the first `Ns` parameters; i.e., $\text{plist}_i = i$ $(i = 0, \ldots, N_s - 1)$.
    If the user provides a function to evaluate the sensitivity residuals, `plist` need not be specified.

    •Parameter scaling factors (optional)
    If IDAS is to estimate tolerances for the sensitivity solution vectors (based on tolerances for the state solution vector) or if IDAS is to evaluate the residuals of the sensitivity systems using the internal difference-quotient function, the results will be more accurate if order of magnitude information is provided.
    Set `pbar`, an array of `Ns` positive scaling factors. Typically, if $p_i \neq 0$, the value $\bar{p}_i = |p_{\text{plist}_i}|$ can be used.
    If `pbar` is not specified, IDAS will use $\bar{p}_i = 1.0$.
    If the user provides a function to evaluate the sensitivity residual and specifies tolerances for the sensitivity variables, `pbar` need not be specified.

    Note that the names for `p`, `pbar`, `plist`, as well as the field p of `user_data` are arbitrary, but they must agree with the arguments passed to `IDASetSensParams` below.

12. **Set sensitivity initial conditions**

    Set the `Ns` vectors `yS0[i]` and `ypS0[i]` of initial values for sensitivities (for $i = 0, \ldots,$ `Ns` -1), using the appropriate functions defined by the particular NVECTOR implementation chosen.

    First, create an array of `Ns` vectors by making the appropriate call

    ```
    yS0 = N_VCloneVectorArray_***(Ns, y0);
    ```

    or

    ```
    yS0 = N_VCloneVectorArrayEmpty_***(Ns, y0);
    ```

    Here the argument `y0` serves only to provide the `N_Vector` type for cloning.

    Then, for each $i = 0, \ldots,$`Ns` -1, load initial values for the i-th sensitivity vector `yS0[i]`.

    Set the initial conditions for the `Ns` sensitivity derivative vectors `ypS0` of $\dot{y}$ similarly.

13. **Activate sensitivity calculations**

    Call `flag = IDASensInit(...);` to activate forward sensitivity computations and allocate internal memory for IDAS related to sensitivity calculations (see §5.2.1).

14. **Set sensitivity tolerances**

    Call `IDASensSStolerances`, `IDASensSVtolerances`, or `IDASensEEtolerances`. See §5.2.2.

15. **Set sensitivity analysis optional inputs**

    Call `IDASetSens*` routines to change from their default values any optional inputs that control the behavior of IDAS in computing forward sensitivities. See §5.2.6.

16. Correct initial values

17. Specify rootfinding problem

18. Advance solution in time

19. **Extract sensitivity solution**

    After each successful return from `IDASolve`, the solution of the original IVP is available in the `y` argument of `IDASolve`, while the sensitivity solution can be extracted into `yS` and `ypS` (which can be the same as `yS0` and `ypS0`, respectively) by calling one of the following routines: `IDAGetSens`, `IDAGetSens1`, `IDAGetSensDky` or `IDAGetSensDky1` (see §5.2.5).

20. Deallocate memory for solutions vector

21. **Deallocate memory for sensitivity vectors**

    Upon completion of the integration, deallocate memory for the vectors contained in `yS0` and `ypS0`:

    ```
    N_VDestroyVectorArray_***(yS0, Ns);
    ```

    and similarly for `ypS0`.

    If `yS` was created from `realtype` arrays `yS_i`, it is the user's responsibility to also free the space for the arrays `yS_i`, and likewise for `ypS`.

22. **Free user data structure**

23. Free solver memory

24. Free vector specification memory

25. Finalize MPI, if used

5.2 User-callable routines for forward sensitivity analysis

This section describes the IDAS functions, in addition to those presented in §4.5, that are called by the user to set up and solve a forward sensitivity problem.

5.2.1 Forward sensitivity initialization and deallocation functions

Activation of forward sensitivity computation is done by calling `IDASensInit`. The form of the call to this routine is as follows:

`IDASensInit`

Call `flag = IDASensInit(ida_mem, Ns, ism, resS, yS0, ypS0);`

Description The routine `IDASensInit` activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

`Ns` (`int`) the number of sensitivities to be computed.

`ism` (`int`) a flag used to select the sensitivity solution method. Its value can be either `IDA_SIMULTANEOUS` or `IDA_STAGGERED`:

- In the `IDA_SIMULTANEOUS` approach, the state and sensitivity variables are corrected at the same time. If `IDA_NEWTON` was selected as the nonlinear system solution method, this amounts to performing a modified Newton iteration on the combined nonlinear system;
- In the `IDA_STAGGERED` approach, the correction step for the sensitivity variables takes place at the same time for all sensitivity equations, but only after the correction of the state variables has converged and the state variables have passed the local error test;

`resS` (`IDASensResFn`) is the C function which computes the residual of the sensitivity DAE. For full details see §5.3.

`yS0` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities of y.

`ypS0` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities of $\dot{y}$.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASensInit` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_MEM_FAIL`	A memory allocation request has failed.
`IDA_ILL_INPUT`	An input argument to `IDASensInit` has an illegal value.

Notes Passing `resS=NULL` indicates using the default internal difference quotient sensitivity residual routine.

If an error occurred, `IDASensInit` also prints an error message to the file specified by the optional input `errfp`.

In terms of the problem size N, number of sensitivity vectors N_s, and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value: `lenrw` = `lenrw` + (`maxord`+5)$N_s N$
- With `IDASensSVtolerances`: `lenrw` = `lenrw` +$N_s N$

the size of the integer workspace is increased as follows:

- Base value: `leniw` = `leniw` + (`maxord`+5)$N_s N_i$
- With `IDASensSVtolerances`: `leniw` = `leniw` +$N_s N_i$,

where N_i is the number of integer words in one `N_Vector`.

The routine `IDASensReInit`, useful during the solution of a sequence of problems of same size, reinitializes the sensitivity-related internal memory and must follow a call to `IDASensInit` (and maybe a call to `IDAReInit`). The number `Ns` of sensitivities is assumed to be unchanged since the call to `IDASensInit`. The call to the `IDASensReInit` function has the form:

`IDASensReInit`

Call `flag = IDASensReInit(ida_mem, ism, yS0, ypS0);`

Description The routine `IDASensReInit` reinitializes forward sensitivity computations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

`ism` (`int`) a flag used to select the sensitivity solution method. Its value can be either `IDA_SIMULTANEOUS` or `IDA_STAGGERED`.

`yS0` (`N_Vector *`) a pointer to an array of `Ns` variables of type `N_Vector` containing the initial values of the sensitivities of y.

`ypS0` (`N_Vector *`) a pointer to an array of `Ns` variables of type `N_Vector` containing the initial values of the sensitivities of $\dot{y}$.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS` The call to `IDAReInit` was successful.

`IDA_MEM_NULL` The IDAS memory block was not initialized through a previous call to `IDACreate`.

`IDA_NO_SENS` Memory space for sensitivity integration was not allocated through a previous call to `IDASensInit`.

`IDA_ILL_INPUT` An input argument to `IDASensReInit` has an illegal value.

`IDA_MEM_FAIL` A memory allocation request has failed.

Notes All arguments of `IDASensReInit` are the same as those of `IDASensInit`.

If an error occurred, `IDASensReInit` also prints an error message to the file specified by the optional input `errfp`.

To deallocate all forward sensitivity-related memory (allocated in a prior call to `IDASensInit`), the user must call

`IDASensFree`

Call `IDASensFree(ida_mem);`

Description The function `IDASensFree` frees the memory allocated for forward sensitivity computations by a previous call to `IDASensInit`.

Arguments The argument is the pointer to the IDAS memory block (of type `void *`).

Return value The function `IDASensFree` has no return value.

Notes In general, `IDASensFree` need not be called by the user as it is invoked automatically by `IDAFree`.

After a call to `IDASensFree`, forward sensitivity computations can be reactivated only by calling `IDASensInit` again.

To activate and deactivate forward sensitivity calculations for successive IDAS runs, without having to allocate and deallocate memory, the following function is provided:

`IDASensToggleOff`

Call `IDASensToggleOff(ida_mem);`

Description The function `IDASensToggleOff` deactivates forward sensitivity calculations. It does *not* deallocate sensitivity-related memory.

Arguments `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

Return value The return value `flag` of `IDASensToggle` is one of:

`IDA_SUCCESS` `IDASensToggleOff` was successful.

`IDA_MEM_NULL` `ida_mem` was `NULL`.

Notes Since sensitivity-related memory is not deallocated, sensitivities can be reactivated at a later time (using `IDASensReInit`).

5.2.2 Forward sensitivity tolerance specification functions

One of the following three functions must be called to specify the integration tolerances for sensitivities. Note that this call must be made after the call to `IDASensInit`.

`IDASensSStolerances`

Call `flag = IDASensSStolerances(ida_mem, reltolS, abstolS);`

Description The function `IDASensSStolerances` specifies scalar relative and absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
`reltolS` (`realtype`) is the scalar relative error tolerance.
`abstolS` (`realtype*`) is a pointer to an array of length `Ns` containing the scalar absolute error tolerances.

Return value The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASStolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_SENS`	The sensitivity allocation function `IDASensInit` has not been called.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

`IDASensSVtolerances`

Call `flag = IDASensSVtolerances(ida_mem, reltolS, abstolS);`

Description The function `IDASensSVtolerances` specifies scalar relative tolerance and vector absolute tolerances.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
`reltolS` (`realtype`) is the scalar relative error tolerance.
`abstolS` (`N_Vector*`) is an array of `Ns` variables of type `N_Vector`. The `N_Vector` from `abstolS[is]` specifies the vector tolerances for `is`-th sensitivity.

Return value The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASVtolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_SENS`	The sensitivity allocation function `IDASensInit` has not been called.
`IDA_ILL_INPUT`	The relative error tolerance was negative or one of the absolute tolerance vectors had a negative component.

Notes This choice of tolerances is important when the absolute error tolerance needs to be different for each component of any vector `yS[i]`.

`IDASensEEtolerances`

Call `flag = IDASensEEtolerances(ida_mem);`

Description When `IDASensEEtolerances` is called, IDAS will estimate tolerances for sensitivity variables based on the tolerances supplied for states variables and the scaling factors $\bar{p}$.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.

Return value The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASensEEtolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_SENS`	The sensitivity allocation function `IDASensInit` has not been called.

5.2.3 Forward sensitivity initial condition calculation function

IDACalcIC also calculates corrected initial conditions for sensitivity variables of a DAE system. When used for initial conditions calculation of the forward sensitivities, IDACalcIC must be preceded by successful calls to IDASensInit (or IDASensReInit) and should precede the call(s) to IDASolve. For restrictions that apply for initial conditions calculation of the state variables, see §4.5.4.

Calling IDACalcIC is optional. It is only necessary when the initial conditions do not satisfy the sensitivity systems. Even if forward sensitivity analysis was enabled, the call to the initial conditions calculation function IDACalcIC is exactly the same as for state variables.

```
flag = IDACalcIC(ida_mem, icopt, tout1);
```

See §4.5.4 for a list of possible return values.

5.2.4 IDAS solver function

Even if forward sensitivity analysis was enabled, the call to the main solver function IDASolve is exactly the same as in §4.5.6. However, in this case the return value flag can also be one of the following:

IDA_SRES_FAIL	The sensitivity residual function failed in an unrecoverable manner.
IDA_REP_SRES_ERR	The user's residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.

5.2.5 Forward sensitivity extraction functions

If forward sensitivity computations have been initialized by a call to IDASensInit, or reinitialized by a call to IDASensReInit, then IDAS computes both a solution and sensitivities at time t. However, IDASolve will still return only the solutions y and $\dot{y}$ in yret and ypret, respectively. Solution sensitivities can be obtained through one of the following functions:

IDAGetSens

Call `flag = IDAGetSens(ida_mem, &tret, yS);`

Description The function IDAGetSens returns the sensitivity solution vectors after a successful return from IDASolve.

Arguments
- ida_mem (void *) pointer to the memory previously allocated by IDAInit.
- tret (realtype) the time reached by the solver (output).
- yS (N_Vector *) the array of Ns computed forward sensitivity vectors.

Return value The return value flag of IDAGetSens is one of:

IDA_SUCCESS	IDAGetSens was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_SENS	Forward sensitivity analysis was not initialized.
IDA_BAD_DKY	yS is NULL.

Notes Note that the argument tret is an output for this function. Its value will be the same as that returned at the last IDASolve call.

The function IDAGetSensDky computes the k-th derivatives of the interpolating polynomials for the sensitivity variables at time t. This function is called by IDAGetSens with k = 0, but may also be called directly by the user.

IDAGetSensDky

Call `flag = IDAGetSensDky(ida_mem, t, k, dkyS);`

Description The function `IDAGetSensDky` returns derivatives of the sensitivity solution vectors after a successful return from `IDASolve`.

Arguments `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

`t` (`realtype`) specifies the time at which sensitivity information is requested. The time `t` must fall within the interval defined by the last successful step taken by IDAS.

`k` (`int`) order of derivatives.

`dkyS` (`N_Vector *`) array of `Ns` vectors containing the derivatives on output. The space for `dkyS` must be allocated by the user.

Return value The return value `flag` of `IDAGetSensDky` is one of:

`IDA_SUCCESS`	`IDAGetSensDky` succeeded.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.
`IDA_BAD_DKY`	`dkyS` or one of the vectors `dkyS[i]` is `NULL`.
`IDA_BAD_K`	`k` is not in the range $0, 1, ..., klast$.
`IDA_BAD_T`	The time `t` is not in the allowed range.

Forward sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions `IDAGetSens1` and `IDAGetSensDky1`, defined as follows:

IDAGetSens1

Call `flag = IDAGetSens1(ida_mem, &tret, is, yS);`

Description The function `IDAGetSens1` returns the `is`-th sensitivity solution vector after a successful return from `IDASolve`.

Arguments `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

`tret` (`realtype *`) the time reached by the solver (output).

`is` (`int`) specifies which sensitivity vector is to be returned ($0 \leq$`is`$< N_s$).

`yS` (`N_Vector`) the computed forward sensitivity vector.

Return value The return value `flag` of `IDAGetSens1` is one of:

`IDA_SUCCESS`	`IDAGetSens1` was successful.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.
`IDA_BAD_IS`	The index `is` is not in the allowed range.
`IDA_BAD_DKY`	`yS` is `NULL`.
`IDA_BAD_T`	The time `t` is not in the allowed range.

Notes Note that the argument `tret` is an output for this function. Its value will be the same as that returned at the last `IDASolve` call.

IDAGetSensDky1

Call `flag = IDAGetSensDky1(ida_mem, t, k, is, dkyS);`

Description The function `IDAGetSensDky1` returns the `k`-th derivative of the `is`-th sensitivity solution vector after a successful return from `IDASolve`.

Arguments `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

t	(realtype) specifies the time at which sensitivity information is requested. The time t must fall within the interval defined by the last successful step taken by IDAS.
k	(int) order of derivative.
is	(int) specifies the sensitivity derivative vector to be returned ($0 \leq$is$< N_s$).
dkyS	(N_Vector) the vector containing the derivative on output. The space for dkyS must be allocated by the user.

Return value The return value flag of IDAGetSensDky1 is one of:

IDA_SUCCESS	IDAGetQuadDky1 succeeded.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_SENS	Forward sensitivity analysis was not initialized.
IDA_BAD_DKY	dkyS is NULL.
IDA_BAD_IS	The index is is not in the allowed range.
IDA_BAD_K	k is not in the range $0, 1, ..., klast$.
IDA_BAD_T	The time t is not in the allowed range.

5.2.6 Optional inputs for forward sensitivity analysis

Optional input variables that control the computation of sensitivities can be changed from their default values through calls to IDASetSens* functions. Table 5.1 lists all forward sensitivity optional input functions in IDAS which are described in detail in the remainder of this section.

IDASetSensParams

Call `flag = IDASetSensParams(ida_mem, p, pbar, plist);`

Description The function IDASetSensParams specifies problem parameter information for sensitivity calculations.

Arguments

ida_mem	(void *) pointer to the IDAS memory block.
p	(realtype *) a pointer to the array of real problem parameters used to evaluate $F(t, y, \dot{y}, p)$. If non-NULL, p must point to a field in the user's data structure user_data passed to the user's residual function. (See §5.1).
pbar	(realtype *) an array of Ns positive scaling factors. If non-NULL, pbar must have all its components > 0.0. (See §5.1).
plist	(int *) an array of Ns non-negative indices to specify which components of p to use in estimating the sensitivity equations. If non-NULL, plist must have all components ≥ 0. (See §5.1).

Return value The return value flag (of type int) is one of:

IDA_SUCCESS	The optional value has been successfully set.
IDA_MEM_NULL	The ida_mem pointer is NULL.
IDA_NO_SENS	Forward sensitivity analysis was not initialized.
IDA_ILL_INPUT	An argument has an illegal value.

Notes This function must be preceded by a call to IDASensInit.

Table 5.1: Forward sensitivity optional inputs

Optional input	Routine name	Default
Sensitivity scaling factors	IDASetSensParams	NULL
DQ approximation method	IDASetSensDQMethod	centered,0.0
Error control strategy	IDASetSensErrCon	FALSE
Maximum no. of nonlinear iterations	IDASetSensMaxNonlinIters	3

`IDASetSensDQMethod`

Call `flag = IDASetSensDQMethod(ida_mem, DQtype, DQrhomax);`

Description The function `IDASetSensDQMethod` specifies the difference quotient strategy in the case in which the residual of the sensitivity equations are to be computed by IDAS.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`DQtype` (`int`) specifies the difference quotient type and can be either `IDA_CENTERED` or `IDA_FORWARD`.

`DQrhomax` (`realtype`) positive value of the selection parameter used in deciding switching between a simultaneous or separate approximation of the two terms in the sensitivity residual.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_ILL_INPUT` An argument has an illegal value.

Notes If `DQrhomax` $= 0.0$, then no switching is performed. The approximation is done simultaneously using either centered or forward finite differences, depending on the value of `DQtype`. For values of `DQrhomax` ≥ 1.0, the simultaneous approximation is used whenever the estimated finite difference perturbations for states and parameters are within a factor of `DQrhomax`, and the separate approximation is used otherwise. Note that a value `DQrhomax` < 1.0 will effectively disable switching. See §2.5 for more details.

The default value are `DQtype`=`IDA_CENTERED` and `DQrhomax`= 0.0.

`IDASetSensErrCon`

Call `flag = IDASetSensErrCon(ida_mem, errconS);`

Description The function `IDASetSensErrCon` specifies the error control strategy for sensitivity variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`errconS` (`booleantype`) specifies whether sensitivity variables are included (`TRUE`) or not (`FALSE`) in the error control mechanism.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes By default, `errconS` is set to `FALSE`. If `errconS`=`TRUE` then both state variables and sensitivity variables are included in the error tests. If `errconS`=`FALSE` then the sensitivity variables are excluded from the error tests. Note that, in any event, all variables are considered in the convergence tests.

`IDASetSensMaxNonlinIters`

Call `flag = IDASetSensMaxNonlinIters(ida_mem, maxcorS);`

Description The function `IDASetSensMaxNonlinIters` specifies the maximum number of nonlinear solver iterations for sensitivity variables per step.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`maxcorS` (`int`) maximum number of nonlinear solver iterations allowed per step (> 0).

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional value has been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

Notes The default value is 3.

5.2.7 Optional outputs for forward sensitivity analysis

5.2.7.1 Main solver optional output functions

Optional output functions that return statistics and solver performance information related to forward sensitivity computations are listed in Table 5.2 and described in detail in the remainder of this section.

`IDAGetSensNumResEvals`

Call `flag = IDAGetSensNumResEvals(ida_mem, &nfSevals);`

Description The function `IDAGetSensNumResEvals` returns the number of calls to the sensitivity residual function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`nfSevals` (`long int`) number of calls to the sensitivity residual function.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.

`IDAGetNumResEvalsSens`

Call `flag = IDAGetNumResEvalsSens(ida_mem, &nfevalsS);`

Description The function `IDAGetNumResEvalsSEns` returns the number of calls to the user's residual function due to the internal finite difference approximation of the sensitivity residuals.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`nfevalsS` (`long int`) number of calls to the user residual function for sensitivity residuals.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if the internal finite difference approximation routines are used for the evaluation of the sensitivity residuals.

Table 5.2: Forward sensitivity optional outputs

Optional output	Routine name
No. of calls to sensitivity residual function	`IDAGetSensNumResEvals`
No. of calls to residual function for sensitivity	`IDAGetNumResEvalsSens`
No. of sensitivity local error test failures	`IDAGetSensNumErrTestFails`
No. of calls to lin. solv. setup routine for sens.	`IDAGetSensNumLinSolvSetups`
Sensitivity-related statistics as a group	`IDAGetSensStats`
Error weight vector for sensitivity variables	`IDAGetSensErrWeights`
No. of sens. nonlinear solver iterations	`IDAGetSensNumNonlinSolvIters`
No. of sens. convergence failures	`IDAGetSensNumNonlinSolvConvFails`
Sens. nonlinear solver statistics as a group	`IDAGetSensNonlinSolvStats`

`IDAGetSensNumErrTestFails`

Call `flag = IDAGetSensNumErrTestFails(ida_mem, &nSetfails);`

Description The function `IDAGetSensNumErrTestFails` returns the number of local error test failures for the sensitivity variables that have occurred.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nSetfails` (`long int`) number of error test failures.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if the sensitivity variables have been included in the error test (see `IDASetSensErrCon` in §5.2.6). Even in that case, this counter is not incremented if the `ism=IDA_SIMULTANEOUS` sensitivity solution method has been used.

`IDAGetSensNumLinSolvSetups`

Call `flag = IDAGetSensNumLinSolvSetups(ida_mem, &nlinsetupsS);`

Description The function `IDAGetSensNumLinSolvSetups` returns the number of calls to the linear solver setup function due to forward sensitivity calculations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nlinsetupsS` (`long int`) number of calls to the linear solver setup function.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if Newton iteration has been used and staggered sensitivity solution method (`ism=IDA_STAGGERED`) was specified in the call to `IDASensInit` (see §5.2.1).

`IDAGetSensStats`

Call
```
flag = IDAGetSensStats(ida_mem, &nfSevals, &nfevalsS, &nSetfails,
                       &nlinsetupsS);
```

Description The function `IDAGetSensStats` returns all of the above sensitivity-related solver statistics as a group.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nfSevals` (`long int`) number of calls to the sensitivity residual function.
`nfevalsS` (`long int`) number of calls to the user-supplied residual function.
`nSetfails` (`long int`) number of error test failures.
`nlinsetupsS` (`long int`) number of calls to the linear solver setup function.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output values have been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Forward sensitivity analysis was not initialized.

`IDAGetSensErrWeights`

Call `flag = IDAGetSensErrWeights(ida_mem, eSweight);`

Description The function `IDAGetSensErrWeights` returns the sensitivity error weight vectors at the current time. These are the reciprocals of the W_i of (2.7) for the sensitivity variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`eSweight` (`N_Vector_S`) pointer to the array of error weight vectors.

Return value The return value `flag` (of type `int`) is one of:
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS` Forward sensitivity analysis was not initialized.

Notes The user must allocate memory for `eweightS`.

`IDAGetSensNumNonlinSolvIters`

Call `flag = IDAGetSensNumNonlinSolvIters(ida_mem, &nSniters);`

Description The function `IDAGetSensNumNonlinSolvIters` returns the number of nonlinear iterations performed for sensitivity calculations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nSniters` (`long int`) number of nonlinear iterations performed.

Return value The return value `flag` (of type `int`) is one of:
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS` Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if `ism` was `IDA_STAGGERED` in the call to `IDASensInit` (see §5.2.1).

`IDAGetSensNumNonlinSolvConvFails`

Call `flag = IDAGetSensNumNonlinSolvConvFails(ida_mem, &nSncfails);`

Description The function `IDAGetSensNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred for sensitivity calculations.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nSncfails` (`long int`) number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of:
`IDA_SUCCESS` The optional output value has been successfully set.
`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS` Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if `ism` was `IDA_STAGGERED` in the call to `IDASensInit` (see §5.2.1).

`IDAGetSensNonlinSolvStats`

Call `flag = IDAGetSensNonlinSolvStats(ida_mem, &nSniters, &nSncfails);`

Description The function `IDAGetSensNonlinSolvStats` returns the sensitivity-related nonlinear solver statistics as a group.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nSniters` (`long int`) number of nonlinear iterations performed.

`nSncfails` (`long int`) number of nonlinear convergence failures.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS` The optional output values have been successfully set.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_NO_SENS` Forward sensitivity analysis was not initialized.

5.2.7.2 Initial condition calculation optional output functions

The sensitivity consistent initial conditions found by IDAS (after a successful call to `IDACalcIC`) can be obtained by calling the following function:

`IDAGetSensConsistentIC`

Call `flag = IDAGetSensConsistentIC(ida_mem, yyS0_mod, ypS0_mod);`

Description The function `IDAGetSensConsistentIC` returns the corrected initial conditions calculated by `IDACalcIC` for sensitivities variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`yyS0_mod` (`N_Vector *`) a pointer to an array of `Ns` vectors containing consistent sensitivity vectors.

`ypS0_mod` (`N_Vector *`) a pointer to an array of `Ns` vectors containing consistent sensitivity derivative vectors.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS` `IDAGetSensConsistentIC` succeeded.

`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDA_NO_SENS` The function `IDASensInit` has not been previously called.

`IDA_ILL_INPUT` `IDASolve` has been already called.

Notes If the consistent sensitivity vectors or consistent derivative vectors are not desired, pass `NULL` for the corresponding argument.

The user must allocate space for `yyS0_mod` and `ypS0_mod` (if not `NULL`).

5.3 User-supplied routines for forward sensitivity analysis

In addition to the required and optional user-supplied routines described in §4.6, when using IDAS for forward sensitivity analysis, the user has the option of providing a routine that calculates the residual of the sensitivity equations (2.12).

By default, IDAS uses difference quotient approximation routines for the residual of the sensitivity equations. However, IDAS allows the option for user-defined sensitivity residual routines (which also provides a mechanism for interfacing IDAS to routines generated by automatic differentiation).

The user may provide the residuals of the sensitivity equations (2.12), for all sensitivity parameters at once, through a function of type `IDASensResFn` defined by:

`IDASensResFn`

Definition
```
typedef int (*IDASensResFn)(int Ns, realtype t,
                            N_Vector yy, N_Vector yp, N_Vector resval,
                            N_Vector *yS, N_Vector *ypS,
                            N_Vector *resvalS, void *user_data,
                            N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the sensitivity residual for all sensitivity equations. It must compute the vectors $(\partial F/\partial y)s_i(t)+(\partial F/\partial \dot{y})\dot{s}_i(t)+(\partial F/\partial p_i)$ and store them in `resvalS[i]`.

Arguments	`t`	is the current value of the independent variable.
	`yy`	is the current value of the state vector, $y(t)$.
	`yp`	is the current value of $\dot{y}(t)$.
	`resval`	contains the current value F of the original DAE residual.
	`yS`	contains the current values of the sensitivities s_i.
	`ypS`	contains the current values of the sensitivity derivatives $\dot{s}_i$.
	`resvalS`	contains the output sensitivity residual vectors.
	`user_data`	is a pointer to user data.
	`tmp1`	
	`tmp2`	
	`tmp3`	are `N_Vector`s of length N which can be used as temporary storage.
Return value	An `IDASensResFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDA_SRES_FAIL` is returned).	
Notes	There is one situation in which recovery is not possible even if `IDASensResFn` function returns a recoverable error flag. That is when this occurs at the very first call to the `IDASensResFn`, in which case IDAS returns `IDA_FIRST_RES_FAIL`.	

5.4 Integration of quadrature equations depending on forward sensitivities

IDAS provides support for integration of quadrature equations that depends not only on the state variables but also on forward sensitivities.

The following is an overview of the sequence of calls in a user's main program in this situation. Steps that are unchanged from the skeleton program presented in §5.1 are grayed out. See also §4.7.

1. **Initialize parallel or multi-threaded environment**
2. **Set problem dimensions, etc.**
3. **Set vectors of initial values**
4. **Create IDAS object**
5. **Allocate internal memory**
6. **Set optional inputs**
7. **Attach linear solver module**
8. **Set linear solver optional inputs**
9. **Initialize sensitivity-independent quadrature problem**
10. **Define the sensitivity problem**
11. **Set sensitivity initial conditions**
12. **Activate sensitivity calculations**
13. **Set sensitivity analysis optional inputs**
14. **Set vector of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.

15. **Initialize sensitivity-dependent quadrature integration**

    Call `IDAQuadSensInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §5.4.1 for details.

16. **Set optional inputs for sensitivity-dependent quadrature integration**

    Call `IDASetQuadSensErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `IDAQuadSens*tolerances` functions must be called to specify the integration tolerances for quadrature variables. See §5.4.4 for details.

17. **Advance solution in time**

18. **Extract sensitivity-dependent quadrature variables**

    Call `IDAGetQuadSens`, `IDAGetQuadSens1`, `IDAGetQuadSensDky` or `IDAGetQuadSensDky1` to obtain the values of the quadrature variables or their derivatives at the current time. See §5.4.3 for details.

19. **Get optional outputs**

20. **Extract sensitivity solution**

21. **Get sensitivity-dependent quadrature optional outputs**

    Call `IDAGetQuadSens*` functions to obtain optional output related to the integration of sensitivity-dependent quadratures. See §5.4.5 for details.

22. **Deallocate memory for solutions vector**

23. **Deallocate memory for sensitivity vectors**

24. **Deallocate memory for sensitivity-dependent quadrature variables**

25. **Free solver memory**

26. **Finalize MPI, if used**

Note: `IDAQuadSensInit` (step 15 above) can be called and quadrature-related optional inputs (step 16 above) can be set, anywhere between steps 10 and 17.

5.4.1 Sensitivity-dependent quadrature initialization and deallocation

The function `IDAQuadSensInit` activates integration of quadrature equations depending on sensitivities and allocates internal memory related to these calculations. If `rhsQS` is input as `NULL`, then IDAS uses an internal function that computes difference quotient approximations to the functions $\bar{q}_i = (\partial q/\partial y)s_i + (\partial q/\partial \dot{y})\dot{s}_i + \partial q/\partial p_i$, in the notation of (2.10). The form of the call to this function is as follows:

`IDAQuadSensInit`

Call `flag = IDAQuadSensInit(ida_mem, rhsQS, yQS0);`

Description The function `IDAQuadSensInit` provides required problem specifications, allocates internal memory, and initializes quadrature integration.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `rhsQS` (`IDAQuadSensRhsFn`) is the C function which computes f_{QS}, the right-hand side of the sensitivity-dependent quadrature equations (for full details see §5.4.6).
- `yQS0` (`N_Vector *`) contains the initial values of sensitivity-dependent quadratures.

Return value The return value `flag` (of type `int`) will be one of the following:

IDA_SUCCESS	The call to IDAQuadSensInit was successful.
IDA_MEM_NULL	The IDAS memory was not initialized by a prior call to IDACreate.
IDA_MEM_FAIL	A memory allocation request failed.
IDA_NO_SENS	The sensitivities were not initialized by a prior call to IDASensInit.
IDA_ILL_INPUT	The parameter yQS0 is NULL.

Notes Before calling IDAQuadSensInit, the user must enable the sensitivites by calling IDASensInit.

If an error occurred, IDAQuadSensInit also sends an error message to the error handler function.

In terms of the number of quadrature variables N_q and maximum method order maxord, the size of the real workspace is increased as follows:

- Base value: lenrw = lenrw + (maxord+5)N_q
- If IDAQuadSensSVtolerances is called: lenrw = lenrw +$N_q N_s$

and the size of the integer workspace is increased as follows:

- Base value: leniw = leniw + (maxord+5)N_q
- If IDAQuadSensSVtolerances is called: leniw = leniw +$N_q N_s$

The function IDAQuadSensReInit, useful during the solution of a sequence of problems of same size, reinitializes the quadrature related internal memory and must follow a call to IDAQuadSensInit. The number Nq of quadratures as well as the number Ns of sensitivities are assumed to be unchanged from the prior call to IDAQuadSensInit. The call to the IDAQuadSensReInit function has the form:

IDAQuadSensReInit

Call `flag = IDAQuadSensReInit(ida_mem, yQS0);`

Description The function IDAQuadSensReInit provides required problem specifications and reinitializes the sensitivity-dependent quadrature integration.

Arguments ida_mem (void *) pointer to the IDAS memory block.
yQS0 (N_Vector *) contains the initial values of sensitivity-dependent quadratures.

Return value The return value flag (of type int) will be one of the following:

IDA_SUCCESS	The call to IDAQuadSensReInit was successful.
IDA_MEM_NULL	The IDAS memory was not initialized by a prior call to IDACreate.
IDA_NO_SENS	Memory space for the sensitivity calculation was not allocated by a prior call to IDASensInit.
IDA_NO_QUADSENS	Memory space for the sensitivity quadratures integration was not allocated by a prior call to IDAQuadSensInit.
IDA_ILL_INPUT	The parameter yQS0 is NULL.

Notes If an error occurred, IDAQuadSensReInit also sends an error message to the error handler function.

IDAQuadSensFree

Call `IDAQuadSensFree(ida_mem);`

Description The function IDAQuadSensFree frees the memory allocated for sensitivity quadrature integration.

Arguments The argument is the pointer to the IDAS memory block (of type void *).

Return value The function IDAQuadSensFree has no return value.

Notes In general, IDAQuadSensFree need not be called by the user as it is called automatically by IDAFree.

5.4.2 IDAS solver function

Even if quadrature integration was enabled, the call to the main solver function `IDASolve` is exactly the same as in §4.5.6. However, in this case the return value `flag` can also be one of the following:

`IDA_QSRHS_FAIL` The sensitivity quadrature right-hand side function failed in an unrecoverable manner.

`IDA_FIRST_QSRHS_ERR` The sensitivity quadrature right-hand side function failed at the first call.

`IDA_REP_QSRHS_ERR` Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. The `IDA_REP_RES_ERR` will also be returned if the quadrature right-hand side function had repeated recoverable errors during the estimation of an initial step size (assuming the sensitivity quadrature variables are included in the error tests).

5.4.3 Sensitivity-dependent quadrature extraction functions

If sensitivity-dependent quadratures have been initialized by a call to `IDAQuadSensInit`, or reinitialized by a call to `IDAQuadSensReInit`, then IDAS computes a solution, sensitivities, and quadratures depending on sensitivities at time `t`. However, `IDASolve` will still return only the solutions y and $\dot{y}$. Sensitivity-dependent quadratures can be obtained using one of the following functions:

`IDAGetQuadSens`

Call `flag = IDAGetQuadSens(ida_mem, &tret, yQS);`

Description The function `IDAGetQuadSens` returns the quadrature sensitivity solution vectors after a successful return from `IDASolve`.

Arguments
- `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.
- `tret` (`realtype`) the time reached by the solver (output).
- `yQS` (`N_Vector *`) array of `Ns` computed sensitivity-dependent quadrature vectors.

Return value The return value `flag` of `IDAGetQuadSens` is one of:
- `IDA_SUCCESS` `IDAGetQuadSens` was successful.
- `IDA_MEM_NULL` `ida_mem` was NULL.
- `IDA_NO_SENS` Sensitivities were not activated.
- `IDA_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.
- `IDA_BAD_DKY` `yQS` or one of the `yQS[i]` is `NULL`.

The function `IDAGetQuadSensDky` computes the `k`-th derivatives of the interpolating polynomials for the sensitivity-dependent quadrature variables at time `t`. This function is called by `IDAGetQuadSens` with `k = 0`, but may also be called directly by the user.

`IDAGetQuadSensDky`

Call `flag = IDAGetQuadSensDky(ida_mem, t, k, dkyQS);`

Description The function `IDAGetQuadSensDky` returns derivatives of the quadrature sensitivities solution vectors after a successful return from `IDASolve`.

Arguments
- `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.
- `t` (`realtype`) the time at which information is requested. The time `t` must fall within the interval defined by the last successful step taken by IDAS.
- `k` (`int`) order of the requested derivative.
- `dkyQS` (`N_Vector *`) array of `Ns` vectors containing the derivatives. This vector array must be allocated by the user.

Return value The return value `flag` of `IDAGetQuadSensDky` is one of:
- `IDA_SUCCESS` `IDAGetQuadSensDky` succeeded.

IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_SENS	Sensitivities were not activated.
IDA_NO_QUADSENS	Quadratures depending on the sensitivities were not activated.
IDA_BAD_DKY	dkyQS or one of the vectors dkyQS[i] is NULL.
IDA_BAD_K	k is not in the range $0, 1, ..., klast$.
IDA_BAD_T	The time t is not in the allowed range.

Quadrature sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions IDAGetQuadSens1 and IDAGetQuadSensDky1, defined as follows:

IDAGetQuadSens1

Call `flag = IDAGetQuadSens1(ida_mem, &tret, is, yQS);`

Description The function IDAGetQuadSens1 returns the is-th sensitivity of quadratures after a successful return from IDASolve.

Arguments
ida_mem	(void *) pointer to the memory previously allocated by IDAInit.
tret	(realtype) the time reached by the solver (output).
is	(int) specifies which sensitivity vector is to be returned ($0 \leq$is$< N_s$).
yQS	(N_Vector) the computed sensitivity-dependent quadrature vector.

Return value The return value flag of IDAGetQuadSens1 is one of:
IDA_SUCCESS	IDAGetQuadSens1 was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_SENS	Forward sensitivity analysis was not initialized.
IDA_NO_QUADSENS	Quadratures depending on the sensitivities were not activated.
IDA_BAD_IS	The index is is not in the allowed range.
IDA_BAD_DKY	yQS is NULL.

IDAGetQuadSensDky1

Call `flag = IDAGetQuadSensDky1(ida_mem, t, k, is, dkyQS);`

Description The function IDAGetQuadSensDky1 returns the k-th derivative of the is-th sensitivity solution vector after a successful return from IDASolve.

Arguments
ida_mem	(void *) pointer to the memory previously allocated by IDAInit.
t	(realtype) specifies the time at which sensitivity information is requested. The time t must fall within the interval defined by the last successful step taken by IDAS.
k	(int) order of derivative.
is	(int) specifies the sensitivity derivative vector to be returned ($0 \leq$is$< N_s$).
dkyQS	(N_Vector) the vector containing the derivative. The space for dkyQS must be allocated by the user.

Return value The return value flag of IDAGetQuadSensDky1 is one of:
IDA_SUCCESS	IDAGetQuadDky1 succeeded.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_SENS	Forward sensitivity analysis was not initialized.
IDA_NO_QUADSENS	Quadratures depending on the sensitivities were not activated.
IDA_BAD_DKY	dkyQS is NULL.
IDA_BAD_IS	The index is is not in the allowed range.
IDA_BAD_K	k is not in the range $0, 1, ..., klast$.
IDA_BAD_T	The time t is not in the allowed range.

5.4.4 Optional inputs for sensitivity-dependent quadrature integration

IDAS provides the following optional input functions to control the integration of sensitivity-dependent quadrature equations.

`IDASetQuadSensErrCon`

Call `flag = IDASetQuadSensErrCon(ida_mem, errconQS)`

Description The function `IDASetQuadSensErrCon` specifies whether or not the quadrature variables are to be used in the local error control mechanism. If they are, the user must specify the error tolerances for the quadrature variables by calling `IDAQuadSensSStolerances`, `IDAQuadSensSVtolerances`, or `IDAQuadSensEEtolerances`.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `errconQS` (`booleantype`) specifies whether sensitivity quadrature variables are included (`TRUE`) or not (`FALSE`) in the error control mechanism.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.

Notes By default, `errconQS` is set to `FALSE`.

It is illegal to call `IDASetQuadSensErrCon` before a call to `IDAQuadSensInit`.

If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

`IDAQuadSensSStolerances`

Call `flag = IDAQuadSensSVtolerances(ida_mem, reltolQS, abstolQS);`

Description The function `IDAQuadSensSStolerances` specifies scalar relative and absolute tolerances.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `reltolQS` (`realtype`) is the scalar relative error tolerance.
- `abstolQS` (`realtype*`) is a pointer to an array containing the `Ns` scalar absolute error tolerances.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

`IDAQuadSensSVtolerances`

Call `flag = IDAQuadSensSVtolerances(ida_mem, reltolQS, abstolQS);`

Description The function `IDAQuadSensSVtolerances` specifies scalar relative and vector absolute tolerances.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `reltolQS` (`realtype`) is the scalar relative error tolerance.
- `abstolQS` (`N_Vector*`) is an array of `Ns` variables of type `N_Vector`. The `N_Vector` from `abstolS[is]` specifies the vector tolerances for `is`-th quadrature sensitivity.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_NO_QUAD`	Quadrature integration was not initialized.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

`IDAQuadSensEEtolerances`

Call `flag = IDAQuadSensEEtolerances(ida_mem);`

Description The function `IDAQuadSensEEtolerances` specifies that the tolerances for the sensitivity-dependent quadratures should be estimated from those provided for the pure quadrature variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.

Notes When `IDAQuadSensEEtolerances` is used, before calling `IDASolve`, integration of pure quadratures must be initialized (see 4.7.1) and tolerances for pure quadratures must be also specified (see 4.7.4).

5.4.5 Optional outputs for sensitivity-dependent quadrature integration

IDAS provides the following functions that can be used to obtain solver performance information related to quadrature integration.

`IDAGetQuadSensNumRhsEvals`

Call `flag = IDAGetQuadSensNumRhsEvals(ida_mem, &nrhsQSevals);`

Description The function `IDAGetQuadSensNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nrhsQSevals` (`long int`) number of calls made to the user's `rhsQS` function.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_QUADSENS`	Sensitivity-dependent quadrature integration has not been initialized.

`IDAGetQuadSensNumErrTestFails`

Call `flag = IDAGetQuadSensNumErrTestFails(ida_mem, &nQSetfails);`

Description The function `IDAGetQuadSensNumErrTestFails` returns the number of local error test failures due to quadrature variables.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`nQSetfails` (`long int`) number of error test failures due to quadrature variables.

Return value The return value `flag` (of type `int`) is one of:

IDA_SUCCESS	The optional output value has been successfully set.
IDA_MEM_NULL	The ida_mem pointer is NULL.
IDA_NO_QUADSENS	Sensitivity-dependent quadrature integration has not been initialized.

IDAGetQuadSensErrWeights

Call `flag = IDAGetQuadSensErrWeights(ida_mem, eQSweight);`

Description The function IDAGetQuadSensErrWeights returns the quadrature error weights at the current time.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `eQSweight` (`N_Vector *`) array of quadrature error weight vectors at the current time.

Return value The return value `flag` (of type `int`) is one of:

IDA_SUCCESS	The optional output value has been successfully set.
IDA_MEM_NULL	The ida_mem pointer is NULL.
IDA_NO_QUADSENS	Sensitivity-dependent quadrature integration has not been initialized.

Notes The user must allocate memory for `eQSweight`.

If quadratures were not included in the error control mechanism (through a call to IDASetQuadSensErrCon with `errconQS=TRUE`), IDAGetQuadSensErrWeights does not set the `eQSweight` vector.

IDAGetQuadSensStats

Call `flag = IDAGetQuadSensStats(ida_mem, &nrhsQSevals, &nQSetfails);`

Description The function IDAGetQuadSensStats returns the IDAS integrator statistics as a group.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `nrhsQSevals` (`long int`) number of calls to the user's `rhsQS` function.
- `nQSetfails` (`long int`) number of error test failures due to quadrature variables.

Return value The return value `flag` (of type `int`) is one of

IDA_SUCCESS	the optional output values have been successfully set.
IDA_MEM_NULL	the ida_mem pointer is NULL.
IDA_NO_QUADSENS	Sensitivity-dependent quadrature integration has not been initialized.

5.4.6 User-supplied function for sensitivity-dependent quadrature integration

For the integration of sensitivity-dependent quadrature equations, the user must provide a function that defines the right-hand side of the sensitivity quadrature equations. For sensitivities of quadratures (2.10) with integrands q, the appropriate right-hand side functions are given by $\bar{q}_i = (\partial q/\partial y)s_i + (\partial q/\partial \dot{y})\dot{s}_i + \partial q/\partial p_i$. This user function must be of type IDAQuadSensRhsFn, defined as follows:

IDAQuadSensRhsFn

Definition
```
typedef int (*IDAQuadSensRhsFn)(int Ns, realtype t, N_Vector yy,
                                N_Vector yp, N_Vector *yyS, N_Vector *ypS,
                                N_Vector rrQ, N_Vector *rhsvalQS,
                                void *user_data, N_Vector tmp1,
                                N_Vector tmp2, N_Vector tmp3)
```

Purpose This function computes the sensitivity quadrature equation right-hand side for a given value of the independent variable t and state vector y.

Arguments

`Ns`	is the number of sensitivity vectors.
`t`	is the current value of the independent variable.
`yy`	is the current value of the dependent variable vector, $y(t)$.
`yp`	is the current value of the dependent variable vector, $\dot{y}(t)$.
`yyS`	is an array of `Ns` variables of type `N_Vector` containing the dependent sensitivity vectors s_i.
`ypS`	is an array of `Ns` variables of type `N_Vector` containing the dependent sensitivity derivatives $\dot{s}_i$.
`rrQ`	is the current value of the quadrature right-hand side q.
`rhsvalQS`	contains the `Ns` output vectors.
`user_data`	is the `user_data` pointer passed to `IDASetUserData`.
`tmp1`	
`tmp2`	
`tmp3`	are `N_Vector`s which can be used as temporary storage.

Return value An `IDAQuadSensRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDA_QRHS_FAIL` is returned).

Notes Allocation of memory for `rhsvalQS` is automatically handled within IDAS.

Both `yy` and `yp` are of type `N_Vector` and both `yyS` and `ypS` are pointers to an array containing `Ns` vectors of type `N_Vector`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

There is one situation in which recovery is not possible even if `IDAQuadSensRhsFn` function returns a recoverable error flag. That is when this occurs at the very first call to the `IDAQuadSensRhsFn`, in which case IDAS returns `IDA_FIRST_QSRHS_ERR`).

5.5 Note on using partial error control

For some problems, when sensitivities are excluded from the error control test, the behavior of IDAS may appear at first glance to be erroneous. One would expect that, in such cases, the sensitivity variables would not influence in any way the step size selection.

The short explanation of this behavior is that the step size selection implemented by the error control mechanism in IDAS is based on the magnitude of the correction calculated by the nonlinear solver. As mentioned in §5.2.1, even with partial error control selected in the call to `IDASensInit`, the sensitivity variables are included in the convergence tests of the nonlinear solver.

When using the simultaneous corrector method (§2.5), the nonlinear system that is solved at each step involves both the state and sensitivity equations. In this case, it is easy to see how the sensitivity variables may affect the convergence rate of the nonlinear solver and therefore the step size selection. The case of the staggered corrector approach is more subtle. The sensitivity variables at a given step are computed only once the solver for the nonlinear state equations has converged. However, if the nonlinear system corresponding to the sensitivity equations has convergence problems, IDAS will attempt to improve the initial guess by reducing the step size in order to provide a better prediction of the sensitivity variables. Moreover, even if there are no convergence failures in the solution of the sensitivity system, IDAS may trigger a call to the linear solver's setup routine which typically involves reevaluation of Jacobian information (Jacobian approximation in the case of IDADENSE and IDABAND, or preconditioner data in the case of the Krylov solvers). The new Jacobian information will be used by subsequent calls to the nonlinear solver for the state equations and, in this way, potentially affect the step size selection.

When using the simultaneous corrector method it is not possible to decide whether nonlinear solver convergence failures or calls to the linear solver setup routine have been triggered by convergence problems due to the state or the sensitivity equations. When using one of the staggered corrector methods, however, these situations can be identified by carefully monitoring the diagnostic information provided through optional outputs. If there are no convergence failures in the sensitivity nonlinear solver, and none of the calls to the linear solver setup routine were made by the sensitivity nonlinear solver, then the step size selection is not affected by the sensitivity variables.

Finally, the user must be warned that the effect of appending sensitivity equations to a given system of DAEs on the step size selection (through the mechanisms described above) is problem-dependent and can therefore lead to either an increase or decrease of the total number of steps that IDAS takes to complete the simulation. At first glance, one would expect that the impact of the sensitivity variables, if any, would be in the direction of increasing the step size and therefore reducing the total number of steps. The argument for this is that the presence of the sensitivity variables in the convergence test of the nonlinear solver can only lead to additional iterations (and therefore a smaller iteration error), or to additional calls to the linear solver setup routine (and therefore more up-to-date Jacobian information), both of which will lead to larger steps being taken by IDAS. However, this is true only locally. Overall, a larger integration step taken at a given time may lead to step size reductions at later times, due to either nonlinear solver convergence failures or error test failures.

Chapter 6

Using IDAS for Adjoint Sensitivity Analysis

This chapter describes the use of IDAS to compute sensitivities of derived functions using adjoint sensitivity analysis. As mentioned before, the adjoint sensitivity module of IDAS provides the infrastructure for integrating backward in time any system of DAEs that depends on the solution of the original IVP, by providing various interfaces to the main IDAS integrator, as well as several supporting user-callable functions. For this reason, in the following sections we refer to the *backward problem* and not to the *adjoint problem* when discussing details relevant to the DAEs that are integrated backward in time. The backward problem can be the adjoint problem (2.20) or (2.25), and can be augmented with some quadrature differential equations.

IDAS uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in Appendix B.

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable functions and of the user-supplied functions that were not already described in Chapter 4.

6.1 A skeleton of the user's main program

The following is a skeleton of the user's main program as an application of IDAS. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the NVECTOR implementation used. Where this is not the case, refer to Chapter 7 for specific names. Steps that are unchanged from the skeleton programs presented in §4.4, §5.1, and §5.4, are grayed out.

1. **Include necessary header files**

   The `idas.h` header file also defines additional types, constants, and function prototypes for the adjoint sensitivity module user-callable functions. In addition, the main program should include an NVECTOR implementation header file (for the particular implementation used) and, if Newton iteration was selected, the main header file of the desired linear solver module.

2. **Initialize parallel or multi-threaded environment**

Forward problem

3. **Set problem dimensions etc. for the forward problem**

4. **Set initial conditions for the forward problem**

5. **Create IDAS object for the forward problem**

6. **Allocate internal memory for the forward problem**
7. **Specify integration tolerances for forward problem**
8. **Set optional inputs for the forward problem**
9. **Attach linear solver module for the forward problem**
10. **Set linear solver optional inputs for the forward problem**
11. **Initialize quadrature problem or problems for forward problems, using `IDAQuadInit` and/or `IDAQuadSensInit`.**
12. **Initialize forward sensitivity problem**
13. **Specify rootfinding**
14. **Allocate space for the adjoint computation**

    Call `IDAAdjInit()` to allocate memory for the combined forward-backward problem (see §6.2.1 for details). This call requires `Nd`, the number of steps between two consecutive checkpoints. `IDAAdjInit` also specifies the type of interpolation used (see §2.6.3).

15. **Integrate forward problem**

    Call `IDASolveF`, a wrapper for the IDAS main integration function `IDASolve`, either in `IDA_NORMAL` mode to the time `tout` or in `IDA_ONE_STEP` mode inside a loop (if intermediate solutions of the forward problem are desired (see §6.2.3)). The final value of `tret` is then the maximum allowable value for the endpoint T of the backward problem.

Backward problem(s)

16. **Set problem dimensions etc. for the backward problem**

    This generally includes `NB`, the number of variables in the backward problem and possibly the local vector length `NBlocal`.

17. **Set initial values for the backward problem**

    Set the endpoint time `tB0` $= T$, and set the corresponding vectors `yB0` and `ypB0` at which the backward problem starts.

18. **Create the backward problem**

    Call `IDACreateB`, a wrapper for `IDACreate`, to create the IDAS memory block for the new backward problem. Unlike `IDACreate`, the function `IDACreateB` does not return a pointer to the newly created memory block (see §6.2.4). Instead, this pointer is attached to the internal adjoint memory block (created by `IDAAdjInit`) and returns an identifier called `which` that the user must later specify in any actions on the newly created backward problem.

19. **Allocate memory for the backward problem**

    Call `IDAInitB` (or `IDAInitBS`, when the backward problem depends on the forward sensitivities). The two functions are actually wrappers for `IDAInit` and allocate internal memory, specify problem data, and initialize IDAS at `tB0` for the backward problem (see §6.2.4).

20. **Specify integration tolerances for backward problem**

    Call `IDASStolerancesB(...)` or `IDASVtolerancesB(...)` to specify a scalar relative tolerance and scalar absolute tolerance, or a scalar relative tolerance and a vector of absolute tolerances, respectively. The functions are wrappers for `IDASStolerances(...)` and `IDASVtolerances(...)`

but they require an extra argument `which`, the identifier of the backward problem returned by `IDACreateB`. See §6.2.5 for more information.

21. **Set optional inputs for the backward problem**

    Call `IDASet*B` functions to change from their default values any optional inputs that control the behavior of IDAS. Unlike their counterparts for the forward problem, these functions take an extra argument `which`, the identifier of the backward problem returned by `IDACreateB` (see §6.2.9).

22. **Attach linear solver module for the backward problem**

    Initialize the linear solver module for the backward problem by calling the appropriate wrapper function: `IDADenseB`, `IDABandB`, `IDALapackDenseB`, `IDALapackBandB`, `IDAKLUB`, `IDASuperLUMTB`, `IDASpgmrB`, `IDASpbcgB`, or `IDASptfqmrB` (see §6.2.6). Note that it is not required to use the same linear solver module for both the forward and the backward problems; for example, the forward problem could be solved with the IDADENSE linear solver and the backward problem with IDASPGMR.

23. **Initialize quadrature calculation**

    If additional quadrature equations must be evaluated, call `IDAQuadInitB` or `IDAQuadInitBS` (if quadrature depends also on the forward sensitivities) as shown in §6.2.11.1. These functions are wrappers around `IDAQuadInit` and can be used to initialize and allocate memory for quadrature integration. Optionally, call `IDASetQuad*B` functions to change from their default values optional inputs that control the integration of quadratures during the backward phase.

24. **Integrate backward problem**

    Call `IDASolveB`, a second wrapper around the IDAS main integration function `IDASolve`, to integrate the backward problem from `tB0` (see §6.2.8). This function can be called either in `IDA_NORMAL` or `IDA_ONE_STEP` mode. Typically, `IDASolveB` will be called in `IDA_NORMAL` mode with an end time equal to the initial time t_0 of the forward problem.

25. **Extract quadrature variables**

    If applicable, call `IDAGetQuadB`, a wrapper around `IDAGetQuad`, to extract the values of the quadrature variables at the time returned by the last call to `IDASolveB`. See §6.2.11.2.

26. **Deallocate memory**

    Upon completion of the backward integration, call all necessary deallocation functions. These include appropriate destructors for the vectors `y` and `yB`, a call to `IDAFree` to free the IDAS memory block for the forward problem. If one or more additional adjoint sensitivity analyses are to be done for this problem, a call to `IDAAdjFree` (see §6.2.1) may be made to free and deallocate the memory allocated for the backward problems, followed by a call to `IDAAdjInit`.

27. **Finalize MPI, if used**

The above user interface to the adjoint sensitivity module in IDAS was motivated by the desire to keep it as close as possible in look and feel to the one for DAE IVP integration. Note that if steps (16)-(25) are not present, a program with the above structure will have the same functionality as one described in §4.4 for integration of DAEs, albeit with some overhead due to the checkpointing scheme.

If there are multiple backward problems associated with the same forward problem, repeat steps (16)-(25) above for each successive backward problem. In the process, each call to `IDACreateB` creates a new value of the identifier `which`.

6.2 User-callable functions for adjoint sensitivity analysis

6.2.1 Adjoint sensitivity allocation and deallocation functions

After the setup phase for the forward problem, but before the call to `IDASolveF`, memory for the combined forward-backward problem must be allocated by a call to the function `IDAAdjInit`. The form of the call to this function is

`IDAAdjInit`

Call `flag = IDAAdjInit(ida_mem, Nd, interpType);`

Description The function `IDAAdjInit` updates IDAS memory block by allocating the internal memory needed for backward integration. Space is allocated for the `Nd` $= N_d$ interpolation data points, and a linked list of checkpoints is initialized.

Arguments
- `ida_mem` (`void *`) is the pointer to the IDAS memory block returned by a previous call to `IDACreate`.
- `Nd` (`long int`) is the number of integration steps between two consecutive checkpoints.
- `interpType` (`int`) specifies the type of interpolation used and can be `IDA_POLYNOMIAL` or `IDA_HERMITE`, indicating variable-degree polynomial and cubic Hermite interpolation, respectively (see §2.6.3).

Return value The return value `flag` (of type `int`) is one of:
- `IDA_SUCCESS` `IDAAdjInit` was successful.
- `IDA_MEM_FAIL` A memory allocation request has failed.
- `IDA_MEM_NULL` `ida_mem` was NULL.
- `IDA_ILL_INPUT` One of the parameters was invalid: `Nd` was not positive or `interpType` is not one of the `IDA_POLYNOMIAL` or `IDA_HERMITE`.

Notes The user must set `Nd` so that all data needed for interpolation of the forward problem solution between two checkpoints fits in memory. `IDAAdjInit` attempts to allocate space for (2`Nd`+3) variables of type `N_Vector`.

If an error occurred, `IDAAdjInit` also sends a message to the error handler function.

`IDAAdjReInit`

Call `flag = IDAAdjReInit(ida_mem);`

Description The function `IDAAdjReInit` reinitializes the IDAS memory block for ASA, assuming that the number of steps between check points and the type of interpolation remain unchanged.

Arguments
- `ida_mem` (`void *`) is the pointer to the IDAS memory block returned by a previous call to `IDACreate`.

Return value The return value `flag` (of type `int`) is one of:
- `IDA_SUCCESS` `IDAAdjReInit` was successful.
- `IDA_MEM_NULL` `ida_mem` was NULL.
- `IDA_NO_ADJ` The function `IDAAdjInit` was not previously called.

Notes The list of check points (and associated memory) is deleted.

The list of backward problems is kept. However, new backward problems can be added to this list by calling `IDACreateB`. If a new list of backward problems is also needed, then free the adjoint memory (by calling `IDAAdjFree`) and reinitialize ASA with `IDAAdjInit`.

The IDAS memory for the forward and backward problems can be reinitialized separately by calling `IDAReInit` and `IDAReInitB`, respectively.

`IDAAdjFree`

Call `IDAAdjFree(ida_mem);`

Description The function `IDAAdjFree` frees the memory related to backward integration allocated by a previous call to `IDAAdjInit`.

Arguments The only argument is the IDAS memory block pointer returned by a previous call to `IDACreate`.

Return value The function `IDAAdjFree` has no return value.

Notes This function frees all memory allocated by `IDAAdjInit`. This includes workspace memory, the linked list of checkpoints, memory for the interpolation data, as well as the IDAS memory for the backward integration phase.

Unless one or more further calls to `IDAAdjInit` are to be made, `IDAAdjFree` should not be called by the user, as it is invoked automatically by `IDAFree`.

6.2.2 Adjoint sensitivity optional input

At any time during the integration of the forward problem, the user can disable the checkpointing of the forward sensitivities by calling the following function:

`IDAAdjSetNoSensi`

Call `flag = IDAAdjSetNoSensi(ida_mem);`

Description The function `IDAAdjSetNoSensi` instructs `IDASolveF` not to save checkpointing data for forward sensitivities any more.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

Return value The return `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The call to `IDACreateB` was successful.
`IDA_MEM_NULL`	The `ida_mem` was `NULL`.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.

6.2.3 Forward integration function

The function `IDASolveF` is very similar to the IDAS function `IDASolve` (see §4.5.6) in that it integrates the solution of the forward problem and returns the solution $(y, \dot{y})$. At the same time, however, `IDASolveF` stores checkpoint data every `Nd` integration steps. `IDASolveF` can be called repeatedly by the user. Note that `IDASolveF` is used only for the forward integration pass within an Adjoint Sensitivity Analysis. It is not for use in Forward Sensitivity Analysis; for that, see Chapter 5. The call to this function has the form

`IDASolveF`

Call `flag = IDASolveF(ida_mem, tout, &tret, yret, ypret, itask, &ncheck);`

Description The function `IDASolveF` integrates the forward problem over an interval in t and saves checkpointing data.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`tout`	(`realtype`) the next time at which a computed solution is desired.
`tret`	(`realtype`) the time reached by the solver (output).
`yret`	(`N_Vector`) the computed solution vector y.
`ypret`	(`N_Vector`) the computed solution vector $\dot{y}$.

`itask` (`int`) a flag indicating the job of the solver for the next step. The `IDA_NORMAL` task is to have the solver take internal steps until it has reached or just passed the user-specified `tout` parameter. The solver then interpolates in order to return an approximate value of y(`tout`) and $\dot{y}$(`tout`). The `IDA_ONE_STEP` option tells the solver to take just one internal step and return the solution at the point reached by that step.

`ncheck` (`int`) the number of (internal) checkpoints stored so far.

Return value On return, `IDASolveF` returns vectors `yret`, `ypret` and a corresponding independent variable value $t =$ `tret`, such that `yret` is the computed value of $y(t)$ and `ypret` the value of $\dot{y}(t)$. Additionally, it returns in `ncheck` the number of internal checkpoints saved; the total number of checkpoint intervals is `ncheck`+1. The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.6.

`IDA_SUCCESS`	`IDASolveF` succeeded.
`IDA_TSTOP_RETURN`	`IDASolveF` succeeded by reaching the optional stopping point.
`IDA_ROOT_RETURN`	`IDASolveF` succeeded and found one or more roots. In this case, `tret` is the location of the root. If `nrtfn` > 1, call `IDAGetRootInfo` to see which g_i were found to have a root.
`IDA_NO_MALLOC`	The function `IDAInit` has not been previously called.
`IDA_ILL_INPUT`	One of the inputs to `IDASolveF` is illegal.
`IDA_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tout`.
`IDA_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`IDA_ERR_FAILURE`	Error test failures occurred too many times during one internal time step or occurred with $\|h\| = h_{min}$.
`IDA_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step or occurred with $\|h\| = h_{min}$.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_MEM_FAIL`	A memory allocation request has failed (in an attempt to allocate space for a new checkpoint).

Notes All failure return values are negative and therefore a test `flag`< 0 will trap all `IDASolveF` failures.

At this time, `IDASolveF` stores checkpoint information in memory only. Future versions will provide for a safeguard option of dumping checkpoint data into a temporary file as needed. The data stored at each checkpoint is basically a snapshot of the IDAS internal memory block and contains enough information to restart the integration from that time and to proceed with the same step size and method order sequence as during the forward integration.

In addition, `IDASolveF` also stores interpolation data between consecutive checkpoints so that, at the end of this first forward integration phase, interpolation information is already available from the last checkpoint forward. In particular, if no checkpoints were necessary, there is no need for the second forward integration phase.

It is illegal to change the integration tolerances between consecutive calls to `IDASolveF`, as this information is not captured in the checkpoint data.

6.2.4 Backward problem initialization functions

The functions `IDACreateB` and `IDAInitB` (or `IDAInitBS`) must be called in the order listed. They instantiate an IDAS solver object, provide problem and solution specifications, and allocate internal

memory for the backward problem.

`IDACreateB`

Call `flag = IDACreateB(ida_mem, &which);`

Description The function `IDACreateB` instantiates an IDAS solver object for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `which` (`int`) contains the identifier assigned by IDAS for the newly created backward problem. Any call to `IDA*B` functions requires such an identifier.

Return value The return `flag` (of type `int`) is one of:
- `IDA_SUCCESS` The call to `IDACreateB` was successful.
- `IDA_MEM_NULL` The `ida_mem` was `NULL`.
- `IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
- `IDA_MEM_FAIL` A memory allocation request has failed.

There are two initialization functions for the backward problem – one for the case when the backward problem does not depend on the forward sensitivities, and one for the case when it does. These two functions are described next.

The function `IDAInitB` initializes the backward problem when it does not depend on the forward sensitivities. It is essentially wrapper for `IDAInit` with some particularization for backward integration, as described below.

`IDAInitB`

Call `flag = IDAInitB(ida_mem, which, resB, tB0, yB0, ypB0);`

Description The function `IDAInitB` provides problem specification, allocates internal memory, and initializes the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `resB` (`IDAResFnB`) is the C function which computes fB, the residual of the backward DAE problem. This function has the form `resB(t, y, yp, yB, ypB, resvalB, user_dataB)` (for full details see §6.3.1).
- `tB0` (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem, normally equal to the endpoint of the forward integration.
- `yB0` (`N_Vector`) is the initial value (at $t =$ `tB0`) of the backward solution.
- `ypB0` (`N_Vector`) is the initial derivative value (at $t =$ `tB0`) of the backward solution.

Return value The return `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAInitB` was successful.
- `IDA_NO_MALLOC` The function `IDAInit` has not been previously called.
- `IDA_MEM_NULL` The `ida_mem` was `NULL`.
- `IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
- `IDA_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
- `IDA_ILL_INPUT` The parameter `which` represented an invalid identifier, or one of `yB0`, `ypB0`, `resB` was `NULL`.

Notes The memory allocated by `IDAInitB` is deallocated by the function `IDAAdjFree`.

For the case when backward problem also depends on the forward sensitivities, user must call `IDAInitBS` instead of `IDAInitB`. Only the third argument of each function differs between these functions.

IDAInitBS

Call `flag = IDAInitBS(ida_mem, which, resBS, tB0, yB0, ypB0);`

Description The function `IDAInitBS` provides problem specification, allocates internal memory, and initializes the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `resBS` (`IDAResFnBS`) is the C function which computes fB, the residual or the backward DAE problem. This function has the form `resBS(t, y, yp, yS, ypS, yB, ypB, resvalB, user_dataB)` (for full details see §6.3.2).
- `tB0` (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem.
- `yB0` (`N_Vector`) is the initial value (at $t =$ `tB0`) of the backward solution.
- `ypB0` (`N_Vector`) is the initial derivative value (at $t =$ `tB0`) of the backward solution.

Return value The return `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAInitB` was successful.
- `IDA_NO_MALLOC` The function `IDAInit` has not been previously called.
- `IDA_MEM_NULL` The `ida_mem` was `NULL`.
- `IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
- `IDA_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
- `IDA_ILL_INPUT` The parameter `which` represented an invalid identifier, or one of `yB0`, `ypB0`, `resB` was `NULL`, or sensitivities were not active during the forward integration.

Notes The memory allocated by `IDAInitBS` is deallocated by the function `IDAAdjFree`.

The function `IDAReInitB` reinitializes IDAS for the solution of a series of backward problems, each identified by a value of the parameter `which`. `IDAReInitB` is essentially a wrapper for `IDAReInit`, and so all details given for `IDAReInit` in §4.5.10 apply here. Also, `IDAReInitB` can be called to reinitialize a backward problem even if it has been initialized with the sensitivity-dependent version `IDAInitBS`. Before calling `IDAReInitB` for a new backward problem, call any desired solution extraction functions `IDAGet**` associated with the previous backward problem. The call to the `IDAReInitB` function has the form

IDAReInitB

Call `flag = IDAReInitB(ida_mem, which, tB0, yB0, ypB0)`

Description The function `IDAReInitB` reinitializes an IDAS backward problem.

Arguments
- `ida_mem` (`void *`) pointer to IDAS memory block returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `tB0` (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem.
- `yB0` (`N_Vector`) is the initial value (at $t =$ `tB0`) of the backward solution.
- `ypB0` (`N_Vector`) is the initial derivative value (at $t =$ `tB0`) of the backward solution.

Return value The return value `flag` (of type `int`) will be one of the following:
- `IDA_SUCCESS` The call to `IDAReInitB` was successful.
- `IDA_NO_MALLOC` The function `IDAInit` has not been previously called.
- `IDA_MEM_NULL` The `ida_mem` memory block pointer was `NULL`.
- `IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
- `IDA_BAD_TB0` The final time `tB0` is outside the interval over which the forward problem was solved.

IDA_ILL_INPUT The parameter which represented an invalid identifier, or one of yB0, ypB0 was NULL.

6.2.5 Tolerance specification functions for backward problem

One of the following two functions must be called to specify the integration tolerances for the backward problem. Note that this call must be made after the call to IDAInitB or IDAInitBS.

IDASStolerancesB

Call `flag = IDASStolerances(ida_mem, which, reltolB, abstolB);`

Description The function IDASStolerancesB specifies scalar relative and absolute tolerances.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by IDACreate.
- `which` (`int`) represents the identifier of the backward problem.
- `reltolB` (`realtype`) is the scalar relative error tolerance.
- `abstolB` (`realtype`) is the scalar absolute error tolerance.

Return value The return `flag` (of type `int`) will be one of the following:
- IDA_SUCCESS The call to IDASStolerancesB was successful.
- IDA_MEM_NULL The IDAS memory block was not initialized through a previous call to IDACreate.
- IDA_NO_MALLOC The allocation function IDAInit has not been called.
- IDA_NO_ADJ The function IDAAdjInit has not been previously called.
- IDA_ILL_INPUT One of the input tolerances was negative.

IDASVtolerancesB

Call `flag = IDASVtolerancesB(ida_mem, which, reltolB, abstolB);`

Description The function IDASVtolerancesB specifies scalar relative tolerance and vector absolute tolerances.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by IDACreate.
- `which` (`int`) represents the identifier of the backward problem.
- `reltol` (`realtype`) is the scalar relative error tolerance.
- `abstol` (`N_Vector`) is the vector of absolute error tolerances.

Return value The return `flag` (of type `int`) will be one of the following:
- IDA_SUCCESS The call to IDASVtolerancesB was successful.
- IDA_MEM_NULL The IDAS memory block was not initialized through a previous call to IDACreate.
- IDA_NO_MALLOC The allocation function IDAInit has not been called.
- IDA_NO_ADJ The function IDAAdjInit has not been previously called.
- IDA_ILL_INPUT The relative error tolerance was negative or the absolute tolerance had a negative component.

Notes This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the DAE state vector y.

6.2.6 Linear solver initialization functions for backward problem

All IDAS linear solver modules available for forward problems provide additional specification functions for backward problems. The initialization functions described in §4.5.3 cannot be directly used since the optional user-defined Jacobian-related functions have different prototypes for the backward problem than for the forward problem (see §6.3).

The following wrapper functions can be used to initialize one of the linear solver modules for the backward problem. Their arguments are identical to those of the functions in §4.5.3 with the exception of the additional second argument, `which`, the identifier of the backward problem.

```
flag = IDADenseB(ida_mem, which, nB);
flag = IDABandB(ida_mem, which, nB, mupperB, mlowerB);
flag = IDALapackDenseB(ida_mem, which, nB);
flag = IDALapackBandB(ida_mem, which, nB, mupperB, mlowerB);
flag = IDAKLUB(ida_mem, which, nB, nnzB, sparsetype);
flag = IDASuperLUMTB(ida_mem, which, num_threads, nB, nnzB);
flag = IDASpgmrB(ida_mem, which, maxlB);
flag = IDASpbcgB(ida_mem, which, maxlB);
flag = IDASptfqmrB(ida_mem, which, maxlB);
```

Their return value `flag` (of type `int`) can have any of the return values of their counterparts. If the `ida_mem` argument was `NULL`, `flag` will be `IDADLS_MEM_NULL`, `IDASLS_MEM_NULL` or `IDASPILS_MEM_NULL`. Also, if `which` is not a valid identifier, the functions will return `IDADLS_ILL_INPUT`, `IDASLS_ILL_INPUT` or `IDASPILS_ILL_INPUT`.

6.2.7 Initial condition calculation functions for backward problem

IDAS provides support for calculation of consistent initial conditions for certain backward index-one problems of semi-implicit form through the functions `IDACalcICB` and `IDACalcICBS`. Calling them is optional. It is only necessary when the initial conditions do not satisfy the adjoint system.

The above functions provide the same functionality for backward problems as `IDACalcIC` with parameter `icopt` = `IDA_YA_YDP_INIT` provides for forward problems (see §4.5.4): compute the algebraic components of yB and differential components of $\dot{y}B$, given the differential components of yB. They require that the `IDASetIdB` was previously called to specify the differential and algebraic components.

Both functions require forward solutions at the final time `tB0`. `IDACalcICBS` also needs forward sensitivities at the final time `tB0`.

`IDACalcICB`

Call `flag = IDACalcICB(ida_mem, which, tBout1, N_Vector yfin, N_Vector ypfin);`

Description The function `IDACalcICB` corrects the initial values `yB0` and `ypB0` at time `tB0` for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `which` (`int`) is the identifier of the backward problem.
- `tBout1` (`realtype`) is the first value of t at which a solution will be requested (from `IDASolveB`). This value is needed here only to determine the direction of integration and rough scale in the independent variable t.
- `yfin` (`N_Vector`) the forward solution at the final time `tB0`.
- `ypfin` (`N_Vector`) the forward solution derivative at the final time `tB0`.

Return value The return value `flag` (of type `int`) can be any that is returned by `IDACalcIC` (see §4.5.4). However `IDACalcICB` can also return one of the following:

`IDA_NO_ADJ`	`IDAAdjInit` has not been previously called.
`IDA_ILL_INPUT`	Parameter `which` represented an invalid identifier.

Notes All failure return values are negative and therefore a test `flag` < 0 will trap all `IDACalcICB` failures.

Note that `IDACalcICB` will correct the values of $yB(tB_0)$ and $\dot{y}B(tB_0)$ which were specified in the previous call to `IDAInitB` or `IDAReInitB`. To obtain the corrected values, call `IDAGetconsistentICB` (see §6.2.10.2).

In the case where the backward problem also depends on the forward sensitivities, user must call the following function to correct the initial conditions:

`IDACalcICBS`

Call `flag = IDACalcICBS(ida_mem, which, tBout1, N_Vector yfin, N_Vector ypfin, N_Vector ySfin, N_Vector ypSfin);`

Description The function `IDACalcICBS` corrects the initial values `yB0` and `ypB0` at time `tB0` for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `which` (`int`) is the identifier of the backward problem.
- `tBout1` (`realtype`) is the first value of t at which a solution will be requested (from `IDASolveB`).This value is needed here only to determine the direction of integration and rough scale in the independent variable t.
- `yfin` (`N_Vector`) the forward solution at the final time `tB0`.
- `ypfin` (`N_Vector`) the forward solution derivative at the final time `tB0`.
- `ySfin` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution at the final time `tB0`.
- `ypSfin` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the derivatives of the forward solution sensitivities at the final time `tB0`.

Return value The return value `flag` (of type `int`) can be any that is returned by `IDACalcIC` (see §4.5.4). However `IDACalcICBS` can also return one of the following:
- `IDA_NO_ADJ` `IDAAdjInit` has not been previously called.
- `IDA_ILL_INPUT` Parameter `which` represented an invalid identifier, sensitivities were not active during forward integration, or `IDAInitBS` (or `IDAReInitBS`) has not been previously called.

Notes All failure return values are negative and therefore a test `flag` < 0 will trap all `IDACalcICBS` failures.

Note that `IDACalcICBS` will correct the values of $yB(tB_0)$ and $\dot{y}B(tB_0)$ which were specified in the previous call to `IDAInitBS` or `IDAReInitBS`. To obtain the corrected values, call `IDAGetConsistentICB` (see §6.2.10.2).

6.2.8 Backward integration function

The function `IDASolveB` performs the integration of the backward problem. It is essentially a wrapper for the IDAS main integration function `IDASolve` and, in the case in which checkpoints were needed, it evolves the solution of the backward problem through a sequence of forward-backward integration pairs between consecutive checkpoints. In each pair, the first run integrates the original IVP forward in time and stores interpolation data; the second run integrates the backward problem backward in time and performs the required interpolation to provide the solution of the IVP to the backward problem.

The function `IDASolveB` does not return the solution `yB` itself. To obtain that, call the function `IDAGetB`, which is also described below.

The `IDASolveB` function does not support rootfinding, unlike `IDASoveF`, which supports the finding of roots of functions of $(t, y, \dot{y})$. If rootfinding was performed by `IDASolveF`, then for the sake of efficiency, it should be disabled for `IDASolveB` by first calling `IDARootInit` with `nrtfn` $= 0$.

The call to `IDASolveB` has the form

`IDASolveB`

Call `flag = IDASolveB(ida_mem, tBout, itaskB);`

Description The function `IDASolveB` integrates the backward DAE problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
- `tBout` (`realtype`) the next time at which a computed solution is desired.
- `itaskB` (`int`) a flag indicating the job of the solver for the next step. The `IDA_NORMAL` task is to have the solver take internal steps until it has reached or just passed the user-specified value `tBout`. The solver then interpolates in order to return an approximate value of yB(`tBout`). The `IDA_ONE_STEP` option tells the solver to take just one internal step in the direction of `tBout` and return.

Return value The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.6.

`IDA_SUCCESS`	`IDASolveB` succeeded.
`IDA_MEM_NULL`	The `ida_mem` was `NULL`.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_NO_BCK`	No backward problem has been added to the list of backward problems by a call to `IDACreateB`
`IDA_NO_FWD`	The function `IDASolveF` has not been previously called.
`IDA_ILL_INPUT`	One of the inputs to `IDASolveB` is illegal.
`IDA_BAD_ITASK`	The `itaskB` argument has an illegal value.
`IDA_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tBout`.
`IDA_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`IDA_ERR_FAILURE`	Error test failures occurred too many times during one internal time step.
`IDA_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_SOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`IDA_BCKMEM_NULL`	The IDAS memory for the backward problem was not created with a call to `IDACreateB`.
`IDA_BAD_TBOUT`	The desired output time `tBout` is outside the interval over which the forward problem was solved.
`IDA_REIFWD_FAIL`	Reinitialization of the forward problem failed at the first checkpoint (corresponding to the initial time of the forward problem).
`IDA_FWD_FAIL`	An error occurred during the integration of the forward problem.

Notes All failure return values are negative and therefore a test `flag`< 0 will trap all `IDASolveB` failures.

In the case of multiple checkpoints and multiple backward problems, a given call to `IDASolveB` in `IDA_ONE_STEP` mode may not advance every problem one step, depending on the relative locations of the current times reached. But repeated calls will eventually advance all problems to `tBout`.

To obtain the solution `yB` to the backward problem, call the function `IDAGetB` as follows:

`IDAGetB`

Call `flag = IDAGetB(ida_mem, which, &tret, yB, ypB);`

Description The function `IDAGetB` provides the solution `yB` of the backward DAE problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
- `which` (`int`) the identifier of the backward problem.
- `tret` (`realtype`) the time reached by the solver (output).

yB	(N_Vector) the backward solution at time tret.
ypB	(N_Vector) the backward solution derivative at time tret.

Return value The return value flag (of type int) will be one of the following.

IDA_SUCCESS	IDAGetB was successful.
IDA_MEM_NULL	ida_mem is NULL.
IDA_NO_ADJ	The function IDAAdjInit has not been previously called.
IDA_ILL_INPUT	The parameter which is an invalid identifier.

Notes The user must allocate space for yB and ypB.

6.2.9 Optional input functions for the backward problem

6.2.9.1 Main solver optional input functions

The adjoint module in IDAS provides wrappers for most of the optional input functions defined in §4.5.7.1. The only difference is that the user must specify the identifier which of the backward problem within the list managed by IDAS.

The optional input functions defined for the backward problem are:

```
flag = IDASetUserDataB(ida_mem, which, user_dataB);
flag = IDASetMaxOrdB(ida_mem, which, maxordB);
flag = IDASetMaxNumStepsB(ida_mem, which, mxstepsB);
flag = IDASetInitStepB(ida_mem, which, hinB)
flag = IDASetMaxStepB(ida_mem, which, hmaxB);
flag = IDASetSuppressAlgB(ida_mem, which, suppressalgB);
flag = IDASetIdB(ida_mem, which, idB);
flag = IDASetConstraintsB(ida_mem, which, constraintsB);
```

Their return value flag (of type int) can have any of the return values of their counterparts, but it can also be IDA_NO_ADJ if IDAAdjInit has not been called, or IDA_ILL_INPUT if which was an invalid identifier.

6.2.9.2 Dense linear solver

Optional inputs for the IDADENSE linear solver module can be set for the backward problem through the following two functions:

IDADlsSetDenseJacFnB

Call `flag = IDADlsSetDenseJacFnB(ida_mem, which, jacB);`

Description The function IDADlsSetDenseJacFnB specifies the dense Jacobian approximation function to be used for the backward problem.

Arguments

ida_mem	(void *) pointer to the IDAS memory returned by IDACreate.
which	(int) represents the identifier of the backward problem.
jacB	(IDADlsDenseJacFnB) user-defined dense Jacobian approximation function.

Return value The return value flag (of type int) is one of:

IDADLS_SUCCESS	IDADlsSetDenseJacFnB succeeded.
IDADLS_MEM_NULL	The ida_mem was NULL.
IDADLS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDADLS_LMEM_NULL	The linear solver has not been initialized with a call to IDADenseB or IDALapackDenseB.
IDADLS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function type IDADlsDenseJacFnB is described in §6.3.5.

`IDADlsSetDenseJacFnBS`

Call `flag = IDADlsSetDenseJacFnBS(ida_mem, which, jacBS);`

Description The function `IDADlsSetDenseJacFnBS` specifies the dense Jacobian approximation function to be used for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `jacBS` (`IDADlsDenseJacFnBS`) user-defined dense Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of:

`IDADLS_SUCCESS`	`IDADlsSetDenseJacFnBS` succeeded.
`IDADLS_MEM_NULL`	The `ida_mem` was `NULL`.
`IDADLS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDADLS_LMEM_NULL`	The linear solver has not been initialized with a call to `IDADenseB` or `IDALapackDenseB`.
`IDADLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `IDADlsDenseJacFnBS` is described in §6.3.5.

6.2.9.3 Band linear solver

Optional inputs for the IDABAND linear solver module can be set for the backward problem through the following two functions:

`IDADlsSetBandJacFnB`

Call `flag = IDADlsSetBandJacFnB(ida_mem, which, jacB);`

Description The function `IDADlsSetBandJacFnB` specifies the banded Jacobian approximation function to be used for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `jacB` (`IDADlsBandJacFnB`) user-defined banded Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of:

`IDADLS_SUCCESS`	`IDADlsSetBandJacFnB` succeeded.
`IDADLS_MEM_NULL`	The `ida_mem` was `NULL`.
`IDADLS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDADLS_LMEM_NULL`	The linear solver has not been initialized with a call to `IDABandB` or `IDALapackBandB`.
`IDADLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `IDADlsBandJacFnB` is described in §6.3.6.

`IDADlsSetBandJacFnBS`

Call `flag = IDADlsSetBandJacFnBS(ida_mem, which, jacBS);`

Description The function `IDADlsSetBandJacFnBS` specifies the banded Jacobian approximation function to be used for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `jacBS` (`IDADlsBandJacFnBS`) user-defined banded Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of:

`IDADLS_SUCCESS`	`IDADlsSetBandJacFnBS` succeeded.
`IDADLS_MEM_NULL`	The `ida_mem` was `NULL`.
`IDADLS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDADLS_LMEM_NULL`	The linear solver has not been initialized with a call to `IDABandB` or `IDALapackBandB`.
`IDADLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `IDADlsBandJacFnBS` is described in §6.3.6.

6.2.9.4 Sparse linear solvers

Optional inputs for the IDAKLU and IDASUPERLUMT linear solver modules can be set for the backward problem through the following functions.

The following wrapper functions can be used to to set the fill-reducing ordering and, in the case of KLU, reinitialize the sparse solver in the sparse linear solver modules for the backward problem. Their arguments are identical to those of the functions in §4.5.3 with the exception of the additional second argument, `which`, the identifier of the backward problem.

```
flag = IDAKLUReInitB(ida_mem, which, nB, nnzB, reinit_typeB);
flag = IDAKLUSetOrderingB(ida_mem, which, ordering_choiceB);
flag = IDASuperLUMTSetOrderingB(ida_mem, which, num_threads, ordering_choiceB);
```

Their return value `flag` (of type `int`) can have any of the return values of their counterparts. If the `ida_mem` argument was `NULL`, `flag` will be `IDASLS_MEM_NULL`. Also, if `which` is not a valid identifier, the functions will return `IDASLS_ILL_INPUT`.

`IDASlsSetSparseJacFnB`

Call `flag = IDASlsSetSparseJacFnB(ida_mem, which, jacB);`

Description The function `IDASlsSetSparseJacFnB` specifies the sparse Jacobian approximation function to be used for the backward problem.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory returned by `IDACreate`.
`which`	(`int`) represents the identifier of the backward problem.
`jacB`	(`IDASlsSparseJacFnB`) user-defined sparse Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of:

`IDASLS_SUCCESS`	`IDASlsSetSparseJacFnB` succeeded.
`IDASLS_MEM_NULL`	The `ida_mem` was `NULL`.
`IDASLS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASLS_LMEM_NULL`	The linear solver has not been initialized with a call to `IDAKLUB` or `IDASuperLUMTB`.
`IDASLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `IDASlsSparseJacFnB` is described in §6.3.7.

`IDASlsSetSparseJacFnBS`

Call `flag = IDASlsSetSparseJacFnBS(ida_mem, which, jacBS);`

Description The function `IDASlsSetSparseJacFnBS` specifies the sparse Jacobian approximation function to be used for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory returned by `IDACreate`.
`which`	(`int`) represents the identifier of the backward problem.

`jacBS` (`IDASlsSparseJacFnBS`) user-defined sparse Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of:

`IDASLS_SUCCESS`	`IDASlsSetSparseJacFnBS` succeeded.
`IDASLS_MEM_NULL`	The `ida_mem` was `NULL`.
`IDASLS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASLS_LMEM_NULL`	The linear solver has not been initialized with a call to `IDAKLUB` or `IDASuperLUMTB`.
`IDASLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `IDASlsSparseJacFnBS` is described in §6.3.7.

6.2.9.5 SPILS linear solvers

Optional inputs for the IDASPILS linear solver module can be set for the backward problem through the following functions:

`IDASpilsSetPreconditionerB`

Call `flag = IDASpilsSetPreconditionerB(ida_mem, which, psetupB, psolveB);`

Description The function `IDASpilsSetPrecSolveFnB` specifies the preconditioner setup and solve functions for the backward integration.

Arguments
`ida_mem` (`void *`) pointer to the IDAS memory block.
`which` (`int`) the identifier of the backward problem.
`psetupB` (`IDASpilsPrecSetupFnB`) user-defined preconditioner setup function.
`psolveB` (`IDASpilsPrecSolveFnB`) user-defined preconditioner solve function.

Return value The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` memory block pointer was `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASPILS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function types `IDASpilsPrecSolveFnB` and `IDASpilsPrecSetupFnB` are described in §6.3.9 and §6.3.10, respectively. The `psetupB` argument may be `NULL` if no setup operation is involved in the preconditioner.

`IDASpilsSetPreconditionerBS`

Call `flag = IDASpilsSetPreconditionerBS(ida_mem, which, psetupBS, psolveBS);`

Description The function `IDASpilsSetPrecSolveFnBS` specifies the preconditioner setup and solve functions for the backward integration, in the case where the backward problem depends on the forward sensitivities.

Arguments
`ida_mem` (`void *`) pointer to the IDAS memory block.
`which` (`int`) the identifier of the backward problem.
`psetupBS` (`IDASpilsPrecSetupFnBS`) user-defined preconditioner setup function.
`psolveBS` (`IDASpilsPrecSolveFnBS`) user-defined preconditioner solve function.

Return value The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` memory block pointer was `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.

IDASPILS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDASPILS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function types IDASpilsPrecSolveFnBS and IDASpilsPrecSetupFnBS are described in §6.3.9 and §6.3.10, respectively. The psetupBS argument may be NULL if no setup operation is involved in the preconditioner.

IDASpilsSetJacTimesVecFnB

Call `flag = IDASpilsSetJacTimesVecFnB(ida_mem, which, jtvB);`

Description The function IDASpilsSetJacTimesVecFnB specifies the Jacobian-vector product function to be used.

Arguments
- ida_mem (void *) pointer to the IDAS memory block.
- which (int) the identifier of the backward problem.
- jtvB (IDASpilsJacTimesVecFnB) user-defined Jacobian-vector product function.

Return value The return value flag (of type int) is one of:

IDASPILS_SUCCESS	The optional value has been successfully set.
IDASPILS_MEM_NULL	The ida_mem memory block pointer was NULL.
IDASPILS_LMEM_NULL	The IDASPILS linear solver has not been initialized.
IDASPILS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDASPILS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function type IDASpilsJacTimesVecFnB is described in §6.3.8.

IDASpilsSetJacTimesVecFnBS

Call `flag = IDASpilsSetJacTimesVecFnBS(ida_mem, which, jtvBS);`

Description The function IDASpilsSetJacTimesVecFnBS specifies the Jacobian-vector product function to be used, in the case where the backward problem depends on the forward sensitivities.

Arguments
- ida_mem (void *) pointer to the IDAS memory block.
- which (int) the identifier of the backward problem.
- jtvBS (IDASpilsJacTimesVecFnBS) user-defined Jacobian-vector product function.

Return value The return value flag (of type int) is one of:

IDASPILS_SUCCESS	The optional value has been successfully set.
IDASPILS_MEM_NULL	The ida_mem memory block pointer was NULL.
IDASPILS_LMEM_NULL	The IDASPILS linear solver has not been initialized.
IDASPILS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDASPILS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function type IDASpilsJacTimesVecFnBS is described in §6.3.8.

IDASpilsSetGSTypeB

Call `flag = IDASpilsSetGSType(ida_mem, which, gstypeB);`

Description The function IDASpilsSetGSTypeB specifies the type of Gram-Schmidt orthogonalization to be used with IDASPGMR. This must be one of the enumeration constants MODIFIED_GS or CLASSICAL_GS. These correspond to using modified Gram-Schmidt and classical Gram-Schmidt, respectively.

Arguments
- ida_mem (void *) pointer to the IDAS memory block.
- which (int) the identifier of the backward problem.

`gstypeB` (`int`) type of Gram-Schmidt orthogonalization.

Return value The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	`ida_mem` was `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASPILS_ILL_INPUT`	The parameter `which` represented an invalid identifier or the value of `gstypeB` was not valid.

Notes The default value is `MODIFIED_GS`.

This option is available only with IDASPGMR.

`IDASpilsSetMaxlB`

Call `flag = IDASpilsSetMaxlB(ida_mem, which, maxlB);`

Description The function `IDASpilsSetMaxlB` resets maximum Krylov subspace dimension for the Bi-CGStab or TFQMR methods.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`which` (`int`) the identifier of the backward problem.

`maxlB` (`realtype`) maximum dimension of the Krylov subspace.

Return value The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	`ida_mem` was `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASPILS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The maximum subspace dimension is initially specified in the call to `IDASpbcgB` or `IDASptfqmrB`. The call to `IDASpilsSetMaxlB` is needed only if `maxlB` is being changed from its previous value.

This option is available only for the IDASPBCG and IDASPTFQMR linear solvers.

`IDASpilsSetEpsLinB`

Call `flag = IDASpilsSetEpsLinB(ida_mem, eplifacB);`

Description The function `IDASpilsSetEpsLinB` specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the Newton iteration test constant. (See §2.1).

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`eplifacB` (`realtype`) linear convergence safety factor (>= 0.0).

Return value The return value `flag` (of type `int`) is one of

`IDASPILS_SUCCESS`	The optional value has been successfully set.
`IDASPILS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDASPILS_LMEM_NULL`	The IDASPILS linear solver has not been initialized.
`IDASPILS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDASPILS_ILL_INPUT`	The value of `eplifacB` is negative.

Notes The default value is 0.05.

Passing a value `eplifacB`= 0.0 also indicates using the default value.

6.2.10 Optional output functions for the backward problem

6.2.10.1 Main solver optional output functions

The user of the adjoint module in IDAS has access to any of the optional output functions described in §4.5.9, both for the main solver and for the linear solver modules. The first argument of these `IDAGet*` and `IDA*Get*` functions is the pointer to the IDAS memory block for the backward problem. In order to call any of these functions, the user must first call the following function to obtain this pointer:

`IDAGetAdjIDABmem`

Call `ida_memB = IDAGetAdjIDABmem(ida_mem, which);`

Description The function `IDAGetAdjIDABmem` returns a pointer to the IDAS memory block for the backward problem.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
`which` (`int`) the identifier of the backward problem.

Return value The return value, `ida_memB` (of type `void *`), is a pointer to the IDAS memory for the backward problem.

Notes The user should not modify `ida_memB` in any way.

Optional output calls should pass `ida_memB` as the first argument; thus, for example, to get the number of integration steps: `flag = IDAGetNumSteps(idas_memB,&nsteps)`.

To get values of the *forward* solution during a backward integration, use the following function. The input value of `t` would typically be equal to that at which the backward solution has just been obtained with `IDAGetB`. In any case, it must be within the last checkpoint interval used by `IDASolveB`.

`IDAGetAdjY`

Call `flag = IDAGetAdjY(ida_mem, t, y, yp);`

Description The function `IDAGetAdjY` returns the interpolated value of the forward solution y and its derivative during a backward integration.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
`t` (`realtype`) value of the independent variable at which y is desired (input).
`y` (`N_Vector`) forward solution $y(t)$.
`yp` (`N_Vector`) forward solution derivative $\dot{y}(t)$.

Return value The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	`IDAGetAdjY` was successful.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_GETY_BADT`	The value of `t` was outside the current checkpoint interval.

Notes The user must allocate space for `y` and `yp`.

6.2.10.2 Initial condition calculation optional output function

`IDAGetConsistentICB`

Call `flag = IDAGetConsistentICB(ida_mem, which, yB0_mod, ypB0_mod);`

Description The function `IDAGetConsistentICB` returns the corrected initial conditions for backward problem calculated by `IDACalcICB`.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`which` is the identifier of the backward problem.

`yB0_mod` (`N_Vector`) consistent initial vector.

`ypB0_mod` (`N_Vector`) consistent initial derivative vector.

Return value The return value `flag` (of type `int`) is one of

`IDA_SUCCESS`	The optional output value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDA_NO_ADJ`	`IDAAdjInit` has not been previously called.
`IDA_ILL_INPUT`	Parameter `which` did not refer a valid backward problem identifier.

Notes If the consistent solution vector or consistent derivative vector is not desired, pass `NULL` for the corresponding argument.

The user must allocate space for `yB0_mod` and `ypB0_mod` (if not `NULL`).

6.2.11 Backward integration of quadrature equations

Not only the backward problem but also the backward quadrature equations may or may not depend on the forward sensitivities. Accordingly, one of the `IDAQuadInitB` or `IDAQuadInitBS` should be used to allocate internal memory and to initialize backward quadratures. For any other operation (extraction, optional input/output, reinitialization, deallocation), the same function is called regardless of whether or not the quadratures are sensitivity-dependent.

6.2.11.1 Backward quadrature initialization functions

The function `IDAQuadInitB` initializes and allocates memory for the backward integration of quadrature equations that do not depende on forward sensititvities. It has the following form:

`IDAQuadInitB`

Call `flag = IDAQuadInitB(ida_mem, which, rhsQB, yQB0);`

Description The function `IDAQuadInitB` provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory block.
`which`	(`int`) the identifier of the backward problem.
`rhsQB`	(`IDAQuadRhsFnB`) is the C function which computes fQB, the residual of the backward quadrature equations. This function has the form `rhsQB(t, y, yp, yB, ypB, rhsvalBQ, user_dataB)` (see §6.3.3).
`yQB0`	(`N_Vector`) is the value of the quadrature variables at `tB0`.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDAQuadInitB` was successful.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_MEM_FAIL`	A memory allocation request has failed.
`IDA_ILL_INPUT`	The parameter `which` is an invalid identifier.

The function `IDAQuadInitBS` initializes and allocates memory for the backward integration of quadrature equations that depend on the forward sensitivities.

`IDAQuadInitBS`

Call `flag = IDAQuadInitBS(ida_mem, which, rhsQBS, yQBS0);`

Description The function `IDAQuadInitBS` provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.

`which`	(`int`) the identifier of the backward problem.
`rhsQBS`	(`IDAQuadRhsFnBS`) is the C function which computes $fQBS$, the residual of the backward quadrature equations. This function has the form `rhsQBS(t, y, yp, yS, ypS, yB, ypB, rhsvalBQS, user_dataB)` (see §6.3.4).
`yQBS0`	(`N_Vector`) is the value of the sensitivity-dependent quadrature variables at `tB0`.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDAQuadInitBS` was successful.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_MEM_FAIL`	A memory allocation request has failed.
`IDA_ILL_INPUT`	The parameter `which` is an invalid identifier.

The integration of quadrature equations during the backward phase can be re-initialized by calling the following function. Before calling `IDAQuadReInitB` for a new backward problem, call any desired solution extraction functions `IDAGet**` associated with the previous backward problem.

`IDAQuadReInitB`

Call `flag = IDAQuadReInitB(ida_mem, which, yQB0);`

Description The function `IDAQuadReInitB` re-initializes the backward quadrature integration.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory block.
`which`	(`int`) the identifier of the backward problem.
`yQB0`	(`N_Vector`) is the value of the quadrature variables at `tB0`.

Return value The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDAQuadReInitB` was successful.
`IDA_MEM_NULL`	`ida_mem` was `NULL`.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_MEM_FAIL`	A memory allocation request has failed.
`IDA_NO_QUAD`	Quadrature integration was not activated through a previous call to `IDAQuadInitB`.
`IDA_ILL_INPUT`	The parameter `which` is an invalid identifier.

Notes `IDAQuadReInitB` can be used after a call to either `IDAQuadInitB` or `IDAQuadInitBS`.

6.2.11.2 Backward quadrature extraction function

To extract the values of the quadrature variables at the last return time of `IDASolveB`, IDAS provides a wrapper for the function `IDAGetQuad` (see §4.7.3). The call to this function has the form

`IDAGetQuadB`

Call `flag = IDAGetQuadB(ida_mem, which, &tret, yQB);`

Description The function `IDAGetQuadB` returns the quadrature solution vector after a successful return from `IDASolveB`.

Arguments

`ida_mem`	(`void *`) pointer to the IDAS memory.
`tret`	(`realtype`) the time reached by the solver (output).
`yQB`	(`N_Vector`) the computed quadrature vector.

Return value

Notes T

he user must allocate space for `yQB`. The return value `flag` of `IDAGetQuadB` is one of:

IDA_SUCCESS	IDAGetQuadB was successful.
IDA_MEM_NULL	ida_mem is NULL.
IDA_NO_ADJ	The function IDAAdjInit has not been previously called.
IDA_NO_QUAD	Quadrature integration was not initialized.
IDA_BAD_DKY	yQB was NULL.
IDA_ILL_INPUT	The parameter which is an invalid identifier.

6.2.11.3 Optional input/output functions for backward quadrature integration

Optional values controlling the backward integration of quadrature equations can be changed from their default values through calls to one of the following functions which are wrappers for the corresponding optional input functions defined in §4.7.4. The user must specify the identifier which of the backward problem for which the optional values are specified.

```
flag = IDASetQuadErrConB(ida_mem, which, errconQ);
flag = IDAQuadSStolerancesB(ida_mem, which, reltolQ, abstolQ);
flag = IDAQuadSVtolerancesB(ida_mem, which, reltolQ, abstolQ);
```

Their return value flag (of type int) can have any of the return values of its counterparts, but it can also be IDA_NO_ADJ if the function IDAAdjInit has not been previously called or IDA_ILL_INPUT if the parameter which was an invalid identifier.

Access to optional outputs related to backward quadrature integration can be obtained by calling the corresponding IDAGetQuad* functions (see §4.7.5). A pointer ida_memB to the IDAS memory block for the backward problem, required as the first argument of these functions, can be obtained through a call to the functions IDAGetAdjIDABmem (see §6.2.10).

6.3 User-supplied functions for adjoint sensitivity analysis

In addition to the required DAE residual function and any optional functions for the forward problem, when using the adjoint sensitivity module in IDAS, the user must supply one function defining the backward problem DAE and, optionally, functions to supply Jacobian-related information and one or two functions that define the preconditioner (if one of the IDASPILS solvers is selected) for the backward problem. Type definitions for all these user-supplied functions are given below.

6.3.1 DAE residual for the backward problem

The user must provide a resB function of type IDAResFnB defined as follows:

IDAResFnB

Definition
```
typedef int (*IDAResFnB)(realtype t, N_Vector y, N_Vector yp,
                         N_Vector yB, N_Vector ypB,
                         N_Vector resvalB, void *user_dataB);
```

Purpose This function evaluates the residual of the backward problem DAE system. This could be (2.20) or (2.25).

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the output vector containing the residual for the backward DAE problem.
user_dataB	is a pointer to user data, same as passed to IDASetUserDataB.

Return value An IDAResFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if an unrecoverabl failure occurred (in which case the integration stops and IDASolveB returns IDA_RESFUNC_FAIL).

Notes Allocation of memory for resvalB is handled within IDAS.

The y, yp, yB, ypB, and resvalB arguments are all of type N_Vector, but yB, ypB, and resvalB typically have different internal representations from y and yp. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their N_Vector arguments (see §7.1 and §7.2).

The user_dataB pointer is passed to the user's resB function every time it is called and can be the same as the user_data pointer used for the forward problem.

Before calling the user's resB function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the residual function which will halt the integration and IDASolveB will return IDA_RESFUNC_FAIL.

6.3.2 DAE residual for the backward problem depending on the forward sensitivities

The user must provide a resBS function of type IDAResFnBS defined as follows:

IDAResFnBS

Definition
```
typedef int (*IDAResFnBS)(realtype t, N_Vector y, N_Vector yp,
                          N_Vector *yS, N_Vector *ypS,
                          N_Vector yB, N_Vector ypB,
                          N_Vector resvalB, void *user_dataB);
```

Purpose This function evaluates the residual of the backward problem DAE system. This could be (2.20) or (2.25).

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
ypS	a pointer to an array of Ns vectors containing the derivatives of the forward sensitivities.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the output vector containing the residual for the backward DAE problem.
user_dataB	is a pointer to user data, same as passed to IDASetUserDataB.

Return value An IDAResFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if an unrecoverable error occurred (in which case the integration stops and IDASolveB returns IDA_RESFUNC_FAIL).

Notes Allocation of memory for resvalB is handled within IDAS.

The y, yp, yB, ypB, and resvalB arguments are all of type N_Vector, but yB, ypB, and resvalB typically have different internal representations from y and yp. Likewise

for each yS[i] and ypS[i]. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their N_Vector arguments (see §7.1 and §7.2).

The user_dataB pointer is passed to the user's resBS function every time it is called and can be the same as the user_data pointer used for the forward problem.

Before calling the user's resBS function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the residual function which will halt the integration and IDASolveB will return IDA_RESFUNC_FAIL.

6.3.3 Quadrature right-hand side for the backward problem

The user must provide an fQB function of type IDAQuadRhsFnB defined by

IDAQuadRhsFnB

Definition
```
typedef int (*IDAQuadRhsFnB)(realtype t, N_Vector y, N_Vector yp,
                             N_Vector yB, N_Vector ypB,
                             N_Vector rhsvalBQ, void *user_dataB);
```

Purpose This function computes the quadrature equation right-hand side for the backward problem.

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
rhsvalBQ	is the output vector containing the residual for the backward quadrature equations.
user_dataB	is a pointer to user data, same as passed to IDASetUserDataB.

Return value An IDAQuadRhsFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and IDASolveB returns IDA_QRHSFUNC_FAIL).

Notes Allocation of memory for rhsvalBQ is handled within IDAS.

The y, yp, yB, ypB, and rhsvalBQ arguments are all of type N_Vector, but they typically all have different internal representations. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with repsect to their N_Vector arguments (see §7.1 and §7.2).

The user_dataB pointer is passed to the user's fQB function every time it is called and can be the same as the user_data pointer used for the forward problem.

Before calling the user's fQB function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and IDASolveB will return IDA_QRHSFUNC_FAIL.

6.3.4 Sensitivity-dependent quadrature right-hand side for the backward problem

The user must provide an `fQBS` function of type `IDAQuadRhsFnBS` defined by

`IDAQuadRhsFnBS`

Definition
```
typedef int (*IDAQuadRhsFnBS)(realtype t, N_Vector y, N_Vector yp,
                              N_Vector *yS, N_Vector *ypS,
                              N_Vector yB, N_Vector ypB,
                              N_Vector rhsvalBQS, void *user_dataB);
```

Purpose This function computes the quadrature equation residual for the backward problem.

Arguments

`t`	is the current value of the independent variable.
`y`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yS`	a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
`ypS`	a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`rhsvalBQS`	is the output vector containing the residual for the backward quadrature equations.
`user_dataB`	is a pointer to user data, same as passed to `IDASetUserDataB`.

Return value An `IDAQuadRhsFnBS` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDASolveB` returns `IDA_QRHSFUNC_FAIL`).

Notes Allocation of memory for `rhsvalBQS` is handled within IDAS.

The `y`, `yp`, `yB`, `ypB`, and `rhsvalBQS` arguments are all of type `N_Vector`, but they typically do not all have the same internal representations. Likewise for each `yS[i]` and `ypS[i]`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with repsect to their `N_Vector` arguments (see §7.1 and §7.2).

The `user_dataB` pointer is passed to the user's `fQBS` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `fQBS` function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and `IDASolveB` will return `IDA_QRHSFUNC_FAIL`.

6.3.5 Jacobian information for the backward problem (direct method with dense Jacobian)

If the direct linear solver with dense treatment of the Jacobian is selected for the backward problem (i.e. `IDADenseB` or `IDALapackDenseB` is called in step 22 of §6.1), the user may provide, through a call to `IDADlsSetDenseJacFnB` or `IDADlsSetDenseJacFnBS` (see §6.2.9), a function of one of the following two types:

`IDADlsDenseJacFnB`

Definition
```
typedef int (*IDADlsDenseJacFnB)(sunindextype NeqB, realtype tt,
                                 realtype cjB, N_Vector yy, N_Vector yp,
                                 N_Vector yB, N_Vector ypB,
                                 N_Vector resvalB,
                                 DlsMat JacB, void *user_dataB,
                                 N_Vector tmp1B, N_Vector tmp2B,
                                 N_Vector tmp3B);
```

Purpose This function computes the dense Jacobian of the backward problem (or an approximation to it).

Arguments

`NeqB`	is the backward problem size (number of equations).
`tt`	is the current value of the independent variable.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`JacB`	is the output approximate dense Jacobian matrix.
`user_dataB`	is a pointer to user data — the parameter passed to `IDASetUserDataB`.
`tmp1B`	
`tmp2B`	
`tmp3B`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADlsDenseJacFnB` as temporary storage or work space.

Return value An `IDADlsDenseJacFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDADENSE sets `last_flag` to `IDADLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

Notes A user-supplied dense Jacobian function must load the `NeqB` by `NeqB` dense matrix `JacB` with an approximation to the Jacobian matrix at the point (`tt`,`yy`,`yB`), where `yy` is the solution of the original IVP at time `tt` and `yB` is the solution of the backward problem at the same time. Only nonzero elements need to be loaded into `JacB` as this matrix is set to zero before the call to the Jacobian function. The type of `JacB` is `DlsMat`. The user is referred to §4.6.5 for details regarding accessing a `DlsMat` object.

Before calling the user's `IDADlsDenseJacFnB`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

`IDADlsDenseJacFnBS`

Definition
```
typedef int (*IDADlsDenseJacFnBS)(sunindextype NeqB, realtype tt,
                                  realtype cjB, N_Vector yy, N_Vector yp,
                                  N_Vector *yS, N_Vector *ypS,
                                  N_Vector yB, N_Vector ypB,
                                  N_Vector resvalB,
                                  DlsMat JacB, void *user_dataB,
                                  N_Vector tmp1B, N_Vector tmp2B,
                                  N_Vector tmp3B);
```

Purpose This function computes the dense Jacobian of the backward problem (or an approximation to it), in the case where the backward problem depends on the forward sensitivities.

Arguments

`NeqB`	is the backward problem size (number of equations).
`tt`	is the current value of the independent variable.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yS`	a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
`ypS`	a pointer to an array of `Ns` vectors containing the derivatives of the forward solution sensitivities.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`JacB`	is the output approximate dense Jacobian matrix.
`user_dataB`	is a pointer to user data — the parameter passed to `IDASetUserDataB`.
`tmp1B`	
`tmp2B`	
`tmp3B`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADlsDenseJacFnBS` as temporary storage or work space.

Return value An `IDADlsDenseJacFnBS` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDADENSE sets `last_flag` to `IDADLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

Notes A user-supplied dense Jacobian function must load the `NeqB` by `NeqB` dense matrix `JacB` with an approximation to the Jacobian matrix at the point (`tt`,`yy`,`yS`,`yB`), where `yy` is the solution of the original IVP at time `tt`, `yS` is the array of forward sensitivities at time `tt`, and `yB` is the solution of the backward problem at the same time. Only nonzero elements need to be loaded into `JacB` as this matrix is set to zero before the call to the Jacobian function. The type of `JacB` is `DlsMat`. The user is referred to §4.6.5 for details regarding accessing a `DlsMat` object.

Before calling the user's `IDADlsDenseJacFnBS`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

6.3.6 Jacobian information for the backward problem (direct method with banded Jacobian)

If the direct linear solver with banded treatment of the Jacobian is selected for the backward problem (i.e. `IDABandB` or `IDALapackBandB` is called in step 22 of §6.1), the user may provide, through a call to `IDADlsSetBandJacFnB` or `IDADlsSetBandJacFnBS` (see §6.2.9), a function of one of the following two types:

`IDADlsBandJacFnB`

Definition
```
typedef int (*IDADlsBandJacFnB)(sunindextype NeqB,
                                sunindextype mupperB, sunindextype mlowerB,
                                realtype tt, realtype cjB,
                                N_Vector yy, N_Vector yp,
                                N_Vector yB, N_Vector ypB,
                                N_Vector resvalB, DlsMat JacB,
                                void *user_dataB,
                                N_Vector tmp1B, N_Vector tmp2B,
                                N_Vector tmp3B);
```

Purpose This function computes the banded Jacobian of the backward problem (or a banded approximation to it).

Arguments

`NeqB`	is the backward problem size.
`mlowerB`	
`mupperB`	are the lower and upper half-bandwidth of the Jacobian.
`tt`	is the current value of the independent variable.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`JacB`	is the output approximate band Jacobian matrix.
`user_dataB`	is a pointer to user data — the parameter passed to `IDASetUserDataB`.
`tmp1B`	
`tmp2B`	
`tmp3B`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADlsBandJacFnB` as temporary storage or work space.

Return value An `IDADlsBandJacFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDABAND sets `last_flag` to `IDADLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

Notes A user-supplied band Jacobian function must load the band matrix `JacB` (of type `DlsMat`) with the elements of the Jacobian at the point (`tt`,`yy`,`yB`), where `yy` is the solution of the original IVP at time `tt` and `yB` is the solution of the backward problem at the same time. Only nonzero elements need to be loaded into `JacB` because `JacB` is preset to zero before the call to the Jacobian function. More details on the accessor macros provided for a `DlsMat` object and on the rest of the arguments passed to a function of type `IDADlsBandJacFnB` are given in §4.6.6.

Before calling the user's `IDADlsBandJacFnB`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL` and IDABAND sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

`IDADlsBandJacFnBS`

Definition
```
typedef int (*IDADlsBandJacFnBS)(sunindextype NeqB,
                                 sunindextype mupperB, sunindextype mlowerB,
                                 realtype tt, realtype cjB,
                                 N_Vector yy, N_Vector yp,
                                 N_Vector *yS, N_Vector *ypS,
                                 N_Vector yB, N_Vector ypB,
                                 N_Vector resvalB, DlsMat JacB,
                                 void *user_dataB,
                                 N_Vector tmp1B, N_Vector tmp2B,
                                 N_Vector tmp3B);
```

Purpose This function computes the banded Jacobian of the backward problem (or a banded approximation to it), in the case where the backward problem depends on the forward sensitivities.

Arguments

`NeqB`	is the backward problem size.
`mlowerB`	
`mupperB`	are the lower and upper half-bandwidth of the Jacobian.
`tt`	is the current value of the independent variable.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yS`	a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
`ypS`	a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`JacB`	is the output approximate band Jacobian matrix.
`user_dataB`	is a pointer to user data — the parameter passed to `IDASetUserDataB`.
`tmp1B`	
`tmp2B`	
`tmp3B`	are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDADlsBandJacFnBS` as temporary storage or work space.

Return value An `IDADlsBandJacFnBS` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDABAND sets `last_flag` to `IDADLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `IDASolveB` returns `IDA_LSETUP_FAIL` and IDADENSE sets `last_flag` to `IDADLS_JACFUNC_UNRECVR`).

Notes A user-supplied band Jacobian function must load the band matrix `JacB` (of type `DlsMat`) with the elements of the Jacobian at the point (`tt`,`yy`,`yS`,`yB`), where `yy` is the solution of the original IVP at time `tt`, `yS` is the array of forward sensitivities at time `tt`, and `yB` is the solution of the backward problem at the same time. Only nonzero elements need to be loaded into `JacB` because `JacB` is preset to zero before the call to the Jacobian function. More details on the accessor macros provided for a `DlsMat` object and on the rest of the arguments passed to a function of type `IDADlsBandJacFnBS` are given in §4.6.6.

Before calling the user's `IDADlsBandJacFnBS`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will

halt the integration (IDASolveB returns IDA_LSETUP_FAIL and IDABAND sets last_flag to IDADLS_JACFUNC_UNRECVR).

6.3.7 Jacobian information for the backward problem (direct method with sparse Jacobian)

If the direct linear solver with sparse treatment of the Jacobian is selected for the backward problem (i.e. IDAKLUB or IDASuperLUMTB is called in step 22 of §6.1), the user must provide, through a call to IDASlsSetSparseJacFnB or IDASlsSetSparseJacFnBS (see §6.2.9), a function of one of the following two types:

IDASlsSparseJacFnB

Definition
```
typedef int (*IDASlsSparseJacFnB)(realtype tt, realtype cjB,
                                  N_Vector yy, N_Vector yp,
                                  N_Vector yB, N_Vector ypB,
                                  N_Vector rrB, SlsMat JacB,
                                  void *user_dataB, N_Vector tmp1B,
                                  N_Vector tmp2B, N_Vector tmp3B);
```

Purpose This function computes the sparse Jacobian of the backward problem (or an approximation to it).

Arguments

tt	is the current value of the independent variable.
cjB	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
yy	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
rrB	is the current value of the residual for the backward problem.
JacB	is the output approximate sparse Jacobian matrix.
user_dataB	is a pointer to user data — the parameter passed to IDASetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by IDASlsSparseJacFnB as temporary storage or work space.

Return value An IDASlsSparseJacFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, IDASolveB returns IDA_LSETUP_FAIL and IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_UNRECVR).

Notes A user-supplied sparse Jacobian function must load the compressed-sparse-column matrix JacB with an approximation to the Jacobian matrix at the point (tt,yy,yB), where yy is the solution of the original IVP at time tt and yB is the solution of the backward problem at the same time. Storage for JacB already exists on entry to this function, although the user should ensure that sufficient space is allocated in JacB to hold the nonzero values to be set; if the existing space is insufficient the user may reallocate the data and row index arrays as needed. The type of JacB is SlsMat, and the amount of allocated space is available within the SlsMat structure as NNZ. The SlsMat type is further documented in the Section §11.2. The user is referred to §4.6.7 for details regarding accessing a SlsMat object.

Before calling the user's IDASlsSparseJacFnB, IDAS needs to evaluate (through inter-

polation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (IDASolveB returns IDA_LSETUP_FAIL and IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_UNRECVR).

IDASlsSparseJacFnBS

Definition
```
typedef int (*IDASlsSparseJacFnBS)(realtype tt, realtype cjB,
                                   N_Vector yy, N_Vector yp,
                                   N_Vector *yS, N_Vector *ypS,
                                   N_Vector yB, N_Vector ypB,
                                   N_Vector rrB, SlsMat JacB,
                                   void *user_dataB, N_Vector tmp1B,
                                   N_Vector tmp2B, N_Vector tmp3B);
```

Purpose This function computes the sparse Jacobian of the backward problem (or an approximation to it), in the case where the backward problem depends on the forward sensitivities.

Arguments

tt	is the current value of the independent variable.
cjB	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
yy	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
ypS	a pointer to an array of Ns vectors containing the derivatives of the forward solution sensitivities.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
rrB	is the current value of the residual for the backward problem.
JacB	is the output approximate sparse Jacobian matrix.
user_dataB	is a pointer to user data — the parameter passed to IDASetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by IDASlsSparseJacFnBS as temporary storage or work space.

Return value An IDASlsSparseJacFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, IDASolveB returns IDA_LSETUP_FAIL and IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_UNRECVR).

Notes A user-supplied sparse Jacobian function must load the compressed-sparse-column matrix JacB with an approximation to the Jacobian matrix at the point (tt,yy,yS,yB), where yy is the solution of the original IVP at time tt, yS is the array of forward sensitivities at time tt, and yB is the solution of the backward problem at the same time. Storage for JacB already exists on entry to this function, although the user should ensure that sufficient space is allocated in JacB to hold the nonzero values to be set; if the existing space is insufficient the user may reallocate the data and row index arrays as needed. The type of JacB is SlsMat, and the amount of allocated space is available within the SlsMat structure as NNZ. The SlsMat type is further documented in the Section §11.2. The user is referred to §4.6.7 for details regarding accessing a SlsMat object.

Before calling the user's IDASlsSparseJacFnBS, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (IDASolveB returns IDA_LSETUP_FAIL and IDAKLU or IDASUPERLUMT sets last_flag to IDASLS_JACFUNC_UNRECVR).

6.3.8 Jacobian information for the backward problem (matrix-vector product)

If one of the Krylov iterative linear solvers SPGMR, SPBCGS, or SPTFQMR is selected (IDASp*B is called in step 22 of §6.1), the user may provide a function of one of the following two forms:

IDASpilsJacTimesVecFnB

Definition
```
typedef int (*IDASpilsJacTimesVecFnB)(realtype t,
                                      N_Vector yy, N_Vector yp,
                                      N_Vector yB, N_Vector ypB,
                                      N_Vector resvalB,
                                      N_Vector vB, N_Vector JvB,
                                      realtype cjB, void *user_dataB,
                                      N_Vector tmp1B, N_Vector tmp2B);
```

Purpose This function computes the action of the backward problem Jacobian JB on a given vector vB.

Arguments

t	is the current value of the independent variable.
yy	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the current value of the residual for the backward problem.
vB	is the vector by which the Jacobian must be multiplied.
JvB	is the computed output vector, JB*vB.
cjB	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.
tmp1B	
tmp2B	are pointers to memory allocated for variables of type N_Vector which can be used by IDASpilsJacTimesVecFnB as temporary storage or work space.

Return value The return value of a function of type IDASpilsJtimesFnB should be 0 if successful or nonzero if an error was encountered, in which case the integration is halted.

Notes A user-supplied Jacobian-vector product function must load the vector JvB with the product of the Jacobian of the backward problem at the point (t, y, yB) and the vector vB. Here, y is the solution of the original IVP at time t and yB is the solution of the backward problem at the same time. The rest of the arguments are equivalent to those passed to a function of type IDASpilsJacTimesVecFn (see §4.6.8). If the backward problem is the adjoint of $\dot{y} = f(t, y)$, then this function is to compute $-(\partial f/\partial y)^T v_B$.

IDASpilsJacTimesVecFnBS

Definition
```
typedef int (*IDASpilsJacTimesVecFnBS)(realtype t,
                                       N_Vector yy, N_Vector yp,
                                       N_Vector *yyS, N_Vector *ypS,
                                       N_Vector yB, N_Vector ypB,
                                       N_Vector resvalB,
                                       N_Vector vB, N_Vector JvB,
                                       realtype cjB, void *user_dataB,
                                       N_Vector tmp1B, N_Vector tmp2B);
```

Purpose This function computes the action of the backward problem Jacobian JB on a given vector vB, in the case where the backward problem depends on the forward sensitivities.

Arguments

t	is the current value of the independent variable.
yy	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yyS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
ypS	a pointer to an array of Ns vectors containing the derivatives of the forward sensitivities.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the current value of the residual for the backward problem.
vB	is the vector by which the Jacobian must be multiplied.
JvB	is the computed output vector, JB*vB.
cjB	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.
tmp1B	
tmp2B	are pointers to memory allocated for variables of type N_Vector which can be used by IDASpilsJacTimesVecFnBS as temporary storage or work space.

Return value The return value of a function of type IDASpilsJtimesFnBS should be 0 if successful or nonzero if an error was encountered, in which case the integration is halted.

Notes A user-supplied Jacobian-vector product function must load the vector JvB with the product of the Jacobian of the backward problem at the point (t, y, yB) and the vector vB. Here, y is the solution of the original IVP at time t and yB is the solution of the backward problem at the same time. The rest of the arguments are equivalent to those passed to a function of type IDASpilsJacTimesVecFn (see §4.6.8).

6.3.9 Preconditioning for the backward problem (linear system solution)

If preconditioning is used during integration of the backward problem, then the user must provide a C function to solve the linear system $Pz = r$, where P is a left preconditioner matrix. This function must have one of the following two forms:

IDASpilsPrecSolveFnB

Definition
```
typedef int (*IDASpilsPrecSolveFnB)(realtype t,
                                    N_Vector yy, N_Vector yp,
                                    N_Vector yB, N_Vector ypB,
                                    N_Vector resvalB,
                                    N_Vector rvecB, N_Vector zvecB,
                                    realtype cjB, realtype deltaB,
                                    void *user_dataB, N_Vector tmpB);
```

Purpose This function solves the preconditioning system $Pz = r$ for the backward problem.

Arguments

`t`	is the current value of the independent variable.
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`rvecB`	is the right-hand side vector r of the linear system to be solved.
`zvecB`	is the computed output vector.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`deltaB`	is an input tolerance to be used if an iterative method is employed in the solution.
`user_dataB`	is a pointer to user data — the same as the `user_dataB` parameter passed to the function `IDASetUserDataB`.
`tmpB`	is a pointer to memory allocated for a variable of type `N_Vector` which can be used for work space.

Return value The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

`IDASpilsPrecSolveFnBS`

Definition
```
typedef int (*IDASpilsPrecSolveFnBS)(realtype t,
                                     N_Vector yy, N_Vector yp,
                                     N_Vector *yyS, N_Vector *ypS,
                                     N_Vector yB, N_Vector ypB,
                                     N_Vector resvalB,
                                     N_Vector rvecB, N_Vector zvecB,
                                     realtype cjB, realtype deltaB,
                                     void *user_dataB, N_Vector tmpB);
```

Purpose This function solves the preconditioning system $Pz = r$ for the backward problem, for the case in which the backward problem depends on the forward sensitivities.

Arguments

`t`	is the current value of the independent variable.
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yyS`	a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
`ypS`	a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.

`rvecB`	is the right-hand side vector r of the linear system to be solved.
`zvecB`	is the computed output vector.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`deltaB`	is an input tolerance to be used if an iterative method is employed in the solution.
`user_dataB`	is a pointer to user data — the same as the `user_dataB` parameter passed to the function `IDASetUserDataB`.
`tmpB`	is a pointer to memory allocated for a variable of type `N_Vector` which can be used for work space.

Return value The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

6.3.10 Preconditioning for the backward problem (Jacobian data)

If the user's preconditioner requires that any Jacobian-related data be preprocessed or evaluated, then this needs to be done in a user-supplied C function of one of the following two types:

`IDASpilsPrecSetupFnB`

Definition
```
typedef int (*IDASpilsPrecSetupFnB)(realtype t,
                                    N_Vector yy, N_Vector yp,
                                    N_Vector yB, N_Vector ypB,
                                    N_Vector resvalB,
                                    realtype cjB, void *user_dataB,
                                    N_Vector tmp1B, N_Vector tmp2B,
                                    N_Vector tmp3B);
```

Purpose This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner for the backward problem.

Arguments The arguments of an `IDASpilsPrecSetupFnB` are as follows:

`t`	is the current value of the independent variable.
`yy`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution vector.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`resvalB`	is the current value of the residual for the backward problem.
`cjB`	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
`user_dataB`	is a pointer to user data — the same as the `user_dataB` parameter passed to the function `IDASetUserDataB`.
`tmp1B`	
`tmp2B`	
`tmp3B`	are pointers to memory allocated for vectors which can be used as temporary storage or work space.

Return value The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

IDASpilsPrecSetupFnBS

Definition
```
typedef int (*IDASpilsPrecSetupFnBS)(realtype t,
                                     N_Vector yy, N_Vector yp,
                                     N_Vector *yyS, N_Vector *ypS,
                                     N_Vector yB, N_Vector ypB,
                                     N_Vector resvalB,
                                     realtype cjB, void *user_dataB,
                                     N_Vector tmp1B, N_Vector tmp2B,
                                     N_Vector tmp3B);
```

Purpose This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments The arguments of an IDASpilsPrecSetupFnBS are as follows:

t	is the current value of the independent variable.
yy	is the current value of the forward solution vector.
yp	is the current value of the forward solution vector.
yyS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
ypS	a pointer to an array of Ns vectors containing the derivatives of the forward sensitivities.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the current value of the residual for the backward problem.
cjB	is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to the function IDASetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for vectors which can be used as temporary storage or work space.

Return value The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

6.4 Using the band-block-diagonal preconditioner for backward problems

As on the forward integration phase, the efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. The band-block-diagonal preconditioner module IDABBDPRE, provides interface functions through which it can be used on the backward integration phase.

The adjoint module in IDAS offers an interface to the band-block-diagonal preconditioner module IDABBDPRE described in section §4.8. This generates a preconditioner that is a block-diagonal matrix with each block being a band matrix and can be used with one of the Krylov linear solvers and with the MPI-parallel vector module NVECTOR_PARALLEL.

In order to use the IDABBDPRE module in the solution of the backward problem, the user must define one or two additional functions, described at the end of this section.

6.4.1 Usage of IDABBDPRE for the backward problem

The IDABBDPRE module is initialized by calling the following function, *after* one of the IDASPILS linear solvers has been specified, by calling the appropriate function (see §6.2.6).

`IDABBDPrecInitB`

Call
```
flag = IDABBDPrecInitB(ida_mem, which, NlocalB, mudqB, mldqB,
                       mukeepB, mlkeepB, dqrelyB, GresB, GcommB);
```

Description The function `IDABBDPrecInitB` initializes and allocates memory for the IDABBDPRE preconditioner for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `which` (`int`) the identifier of the backward problem.
- `NlocalB` (`sunindextype`) local vector dimension for the backward problem.
- `mudqB` (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mldqB` (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mukeepB` (`sunindextype`) upper half-bandwidth of the retained banded approximate Jacobian block.
- `mlkeepB` (`sunindextype`) lower half-bandwidth of the retained banded approximate Jacobian block.
- `dqrelyB` (`realtype`) the relative increment in components of `yB` used in the difference quotient approximations. The default is `dqrelyB`$= \sqrt{\text{unit roundoff}}$, which can be specified by passing `dqrely`$= 0.0$.
- `GresB` (`IDABBDLocalFnB`) the C function which computes $G_B(t, y, \dot{y}, y_B, \dot{y}_B)$, the function approximating the residual of the backward problem.
- `GcommB` (`IDABBDCommFnB`) the optional C function which performs all interprocess communication required for the computation of G_B.

Return value If successful, `IDABBDPrecInitB` creates, allocates, and stores (internally in the IDAS solver block) a pointer to the newly created IDABBDPRE memory block. The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The call to `IDABBDPrecInitB` was successful.
`IDASPILS_MEM_FAIL`	A memory allocation request has failed.
`IDASPILS_MEM_NULL`	The `ida_mem` argument was `NULL`.
`IDASPILS_LMEM_NULL`	No linear solver has been attached.
`IDASPILS_ILL_INPUT`	An invalid parameter has been passed.

To reinitialize the IDABBDPRE preconditioner module for the backward problem, possibly with a change in `mudqB`, `mldqB`, or `dqrelyB`, call the following function:

`IDABBDPrecReInitB`

Call
```
flag = IDABBDPrecReInitB(ida_mem, which, mudqB, mldqB, dqrelyB);
```

Description The function `IDABBDPrecReInitB` reinitializes the IDABBDPRE preconditioner for the backward problem.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
- `which` (`int`) the identifier of the backward problem.
- `mudqB` (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
- `mldqB` (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.

`dqrelyB` (`realtype`) the relative increment in components of `yB` used in the difference quotient approximations.

Return value The return value `flag` (of type `int`) is one of:

`IDASPILS_SUCCESS`	The call to `IDABBDPrecReInitB` was successful.
`IDASPILS_MEM_FAIL`	A memory allocation request has failed.
`IDASPILS_MEM_NULL`	The `ida_mem` argument was `NULL`.
`IDASPILS_PMEM_NULL`	The `IDABBDPrecInitB` has not been previously called.
`IDASPILS_LMEM_NULL`	No linear solver has been attached.
`IDASPILS_ILL_INPUT`	An invalid parameter has been passed.

For more details on IDABBDPRE see §4.8.

6.4.2 User-supplied functions for IDABBDPRE

To use the IDABBDPRE module, the user must supply one or two functions which the module calls to construct the preconditioner: a required function `GresB` (of type `IDABBDLocalFnB`) which approximates the residual of the backward problem and which is computed locally, and an optional function `GcommB` (of type `IDABBDCommFnB`) which performs all interprocess communication necessary to evaluate this approximate residual (see §4.8). The prototypes for these two functions are described below.

`IDABBDLocalFnB`

Definition
```
typedef int (*IDABBDLocalFnB)(sunindextype NlocalB, realtype t,
                              N_Vector y, N_Vector yp,
                              N_Vector yB, N_Vector ypB,
                              N_Vector gB, void *user_dataB);
```

Purpose This `GresB` function loads the vector `gB`, an approximation to the residual of the backward problem, as a function of `t`, `y`, `yp`, and `yB` and `ypB`.

Arguments

`NlocalB`	is the local vector length for the backward problem.
`t`	is the value of the independent variable.
`y`	is the current value of the forward solution vector.
`yp`	is the current value of the forward solution derivative vector.
`yB`	is the current value of the backward dependent variable vector.
`ypB`	is the current value of the backward dependent derivative vector.
`gB`	is the output vector, $G_B(t, y, \dot{y}, y_B, \dot{y}_B)$.
`user_dataB`	is a pointer to user data — the same as the `user_dataB` parameter passed to `IDASetUserDataB`.

Return value An `IDABBDLocalFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDASolveB` returns `IDA_LSETUP_FAIL`).

Notes This routine must assume that all interprocess communication of data needed to calculate `gB` has already been done, and this data is accessible within `user_dataB`.

Before calling the user's `IDABBDLocalFnB`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the preconditioner setup function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL`).

IDABBDCommFnB

Definition
```
typedef int (*IDABBDCommFnB)(sunindextype NlocalB, realtype t,
                             N_Vector y, N_Vector yp,
                             N_Vector yB, N_Vector ypB,
                             void *user_dataB);
```

Purpose This GcommB function performs all interprocess communications necessary for the execution of the GresB function above, using the input vectors y, yp, yB and ypB.

Arguments

NlocalB	is the local vector length.
t	is the value of the independent variable.
y	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.

Return value An IDABBDCommFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and IDASolveB returns IDA_LSETUP_FAIL).

Notes The GcommB function is expected to save communicated data in space defined within the structure user_dataB.

Each call to the GcommB function is preceded by a call to the function that evaluates the residual of the backward problem with the same t, y, yp, yB and ypB arguments. If there is no additional communication needed, then pass GcommB = NULL to IDABBDPrecInitB.

Chapter 7

Description of the NVECTOR module

The SUNDIALS solvers are written in a data-independent manner. They all operate on generic vectors (of type `N_Vector`) through a set of operations defined by the particular NVECTOR implementation. Users can provide their own specific implementation of the NVECTOR module, or use one of four provided within SUNDIALS – a serial implementation and three parallel implementations. The generic operations are described below. In the sections following, the implementations provided with SUNDIALS are described.

The generic `N_Vector` type is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the vector, and an *ops* field pointing to a structure with generic vector operations. The type `N_Vector` is defined as

```
typedef struct _generic_N_Vector *N_Vector;

struct _generic_N_Vector {
    void *content;
    struct _generic_N_Vector_Ops *ops;
};
```

The `_generic_N_Vector_Ops` structure is essentially a list of pointers to the various actual vector operations, and is defined as

```
struct _generic_N_Vector_Ops {
  N_Vector_ID (*nvgetvectorid)(N_Vector);
  N_Vector    (*nvclone)(N_Vector);
  N_Vector    (*nvcloneempty)(N_Vector);
  void        (*nvdestroy)(N_Vector);
  void        (*nvspace)(N_Vector, sunindextype *, sunindextype *);
  realtype*   (*nvgetarraypointer)(N_Vector);
  void        (*nvsetarraypointer)(realtype *, N_Vector);
  void        (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
  void        (*nvconst)(realtype, N_Vector);
  void        (*nvprod)(N_Vector, N_Vector, N_Vector);
  void        (*nvdiv)(N_Vector, N_Vector, N_Vector);
  void        (*nvscale)(realtype, N_Vector, N_Vector);
  void        (*nvabs)(N_Vector, N_Vector);
  void        (*nvinv)(N_Vector, N_Vector);
  void        (*nvaddconst)(N_Vector, realtype, N_Vector);
  realtype    (*nvdotprod)(N_Vector, N_Vector);
  realtype    (*nvmaxnorm)(N_Vector);
```

```
  realtype    (*nvwrmsnorm)(N_Vector, N_Vector);
  realtype    (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
  realtype    (*nvmin)(N_Vector);
  realtype    (*nvwl2norm)(N_Vector, N_Vector);
  realtype    (*nvl1norm)(N_Vector);
  void        (*nvcompare)(realtype, N_Vector, N_Vector);
  booleantype (*nvinvtest)(N_Vector, N_Vector);
  booleantype (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
  realtype    (*nvminquotient)(N_Vector, N_Vector);
};
```

The generic NVECTOR module defines and implements the vector operations acting on `N_Vector`. These routines are nothing but wrappers for the vector operations defined by a particular NVECTOR implementation, which are accessed through the *ops* field of the `N_Vector` structure. To illustrate this point we show below the implementation of a typical vector operation from the generic NVECTOR module, namely `N_VScale`, which performs the scaling of a vector `x` by a scalar `c`:

```
void N_VScale(realtype c, N_Vector x, N_Vector z)
{
   z->ops->nvscale(c, x, z);
}
```

Table 7.2 contains a complete list of all vector operations defined by the generic NVECTOR module.

Finally, note that the generic NVECTOR module defines the functions `N_VCloneVectorArray` and `N_VCloneVectorArrayEmpty`. Both functions create (by cloning) an array of `count` variables of type `N_Vector`, each of the same type as an existing `N_Vector`. Their prototypes are

```
N_Vector *N_VCloneVectorArray(int count, N_Vector w);
N_Vector *N_VCloneVectorArrayEmpty(int count, N_Vector w);
```

and their definitions are based on the implementation-specific `N_VClone` and `N_VCloneEmpty` operations, respectively.

An array of variables of type `N_Vector` can be destroyed by calling `N_VDestroyVectorArray`, whose prototype is

```
void N_VDestroyVectorArray(N_Vector *vs, int count);
```

and whose definition is based on the implementation-specific `N_VDestroy` operation.

A particular implementation of the NVECTOR module must:

- Specify the *content* field of `N_Vector`.
- Define and implement the vector operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one NVECTOR module (each with different `N_Vector` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free an `N_Vector` with the new *content* field and with *ops* pointing to the new vector operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined `N_Vector` (e.g., a routine to print the content for debugging purposes).
- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the *content* field of the newly defined `N_Vector`.

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 7.1. It is recommended that a user-supplied NVECTOR implementation use the `SUNDIALS_NVEC_CUSTOM` identifier.

Table 7.1: Vector Identifications associated with vector kernels supplied with SUNDIALS.

Vector ID	Vector type	ID Value
SUNDIALS_NVEC_SERIAL	Serial	0
SUNDIALS_NVEC_PARALLEL	Distributed memory parallel (MPI)	1
SUNDIALS_NVEC_OPENMP	OpenMP shared memory parallel	2
SUNDIALS_NVEC_PTHREADS	PThreads shared memory parallel	3
SUNDIALS_NVEC_PARHYP	*hypre* ParHyp parallel vector	4
SUNDIALS_NVEC_PETSC	PETSc parallel vector	5
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	6

Table 7.2: Description of the NVECTOR operations

Name	Usage and Description
`N_VGetVectorID`	`id = N_VGetVectorID(w);` Returns the vector type identifier for the vector `w`. It is used to determine the vector implementation type (e.g. serial, parallel,...) from the abstract `N_Vector` interface. Returned values are given in Table 7.1.
`N_VClone`	`v = N_VClone(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not copy the vector, but rather allocates storage for the new vector.
`N_VCloneEmpty`	`v = N_VCloneEmpty(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not allocate storage for data.
`N_VDestroy`	`N_VDestroy(v);` Destroys the `N_Vector v` and frees memory allocated for its internal data.
`N_VSpace`	`N_VSpace(nvSpec, &lrw, &liw);` Returns storage requirements for one `N_Vector`. `lrw` contains the number of realtype words and `liw` contains the number of integer words. This function is advisory only, for use in determining a user's total space requirements; it could be a dummy function in a user-supplied NVECTOR module if that information is not of interest.

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Name	Usage and Description
N_VGetArrayPointer	`vdata = N_VGetArrayPointer(v);` Returns a pointer to a `realtype` array from the `N_Vector v`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype`. This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, the sparse linear solvers (serial and threaded), and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS.
N_VSetArrayPointer	`N_VSetArrayPointer(vdata, v);` Overwrites the data in an `N_Vector` with a given array of `realtype`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype`. This routine is only used in the interfaces to the dense (serial) linear solver, hence need not exist in a user-supplied NVECTOR module for a parallel environment.
N_VLinearSum	`N_VLinearSum(a, x, b, y, z);` Performs the operation $z = ax + by$, where a and b are `realtype` scalars and x and y are of type `N_Vector`: $z_i = ax_i + by_i$, $i = 0, \ldots, n-1$.
N_VConst	`N_VConst(c, z);` Sets all components of the `N_Vector z` to `realtype c`: $z_i = c$, $i = 0, \ldots, n-1$.
N_VProd	`N_VProd(x, y, z);` Sets the `N_Vector z` to be the component-wise product of the `N_Vector` inputs `x` and `y`: $z_i = x_i y_i$, $i = 0, \ldots, n-1$.
N_VDiv	`N_VDiv(x, y, z);` Sets the `N_Vector z` to be the component-wise ratio of the `N_Vector` inputs `x` and `y`: $z_i = x_i/y_i$, $i = 0, \ldots, n-1$. The y_i may not be tested for 0 values. It should only be called with a `y` that is guaranteed to have all nonzero components.
N_VScale	`N_VScale(c, x, z);` Scales the `N_Vector x` by the `realtype` scalar `c` and returns the result in `z`: $z_i = cx_i$, $i = 0, \ldots, n-1$.
N_VAbs	`N_VAbs(x, z);` Sets the components of the `N_Vector z` to be the absolute values of the components of the `N_Vector x`: $y_i = \lvert x_i \rvert$, $i = 0, \ldots, n-1$.

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Name	Usage and Description
N_VInv	`N_VInv(x, z);` Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine may not check for division by 0. It should be called only with an `x` which is guaranteed to have all nonzero components.
N_VAddConst	`N_VAddConst(x, b, z);` Adds the `realtype` scalar `b` to all components of `x` and returns the result in the `N_Vector z`: $z_i = x_i + b$, $i = 0, \ldots, n-1$.
N_VDotProd	`d = N_VDotProd(x, y);` Returns the value of the ordinary dot product of `x` and `y`: $d = \sum_{i=0}^{n-1} x_i y_i$.
N_VMaxNorm	`m = N_VMaxNorm(x);` Returns the maximum norm of the `N_Vector x`: $m = \max_i \lvert x_i \rvert$.
N_VWrmsNorm	`m = N_VWrmsNorm(x, w)` Returns the weighted root-mean-square norm of the `N_Vector x` with `realtype` weight vector `w`: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i)^2\right)/n}$.
N_VWrmsNormMask	`m = N_VWrmsNormMask(x, w, id);` Returns the weighted root mean square norm of the `N_Vector x` with `realtype` weight vector `w` built using only the elements of `x` corresponding to nonzero elements of the `N_Vector id`: $m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i \mathrm{sign}(id_i))^2\right)/n}$.
N_VMin	`m = N_VMin(x);` Returns the smallest element of the `N_Vector x`: $m = \min_i x_i$.
N_VWL2Norm	`m = N_VWL2Norm(x, w);` Returns the weighted Euclidean ℓ_2 norm of the `N_Vector x` with `realtype` weight vector `w`: $m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}$.
N_VL1Norm	`m = N_VL1Norm(x);` Returns the ℓ_1 norm of the `N_Vector x`: $m = \sum_{i=0}^{n-1} \lvert x_i \rvert$.
N_VCompare	`N_VCompare(c, x, z);` Compares the components of the `N_Vector x` to the `realtype` scalar `c` and returns an `N_Vector z` such that: $z_i = 1.0$ if $\lvert x_i \rvert \geq c$ and $z_i = 0.0$ otherwise.

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Name	**Usage and Description**
N_VInvTest	`t = N_VInvTest(x, z);` Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`, with prior testing for zero values: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine returns a boolean assigned to `TRUE` if all components of `x` are nonzero (successful inversion) and returns `FALSE` otherwise.
N_VConstrMask	`t = N_VConstrMask(c, x, m);` Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \geq 0$ if $c_i = 1$, $x_i \leq 0$ if $c_i = -1$, $x_i < 0$ if $c_i = -2$. There is no constraint on x_i if $c_i = 0$. This routine returns a boolean assigned to `FALSE` if any element failed the constraint test and assigned to `TRUE` if all passed. It also sets a mask vector `m`, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.
N_VMinQuotient	`minq = N_VMinQuotient(num, denom);` This routine returns the minimum of the quotients obtained by termwise dividing $\texttt{num}_i$ by $\texttt{denom}_i$. A zero element in `denom` will be skipped. If no such quotients are found, then the large value `BIG_REAL` (defined in the header file `sundials_types.h`) is returned.

7.1 The NVECTOR_SERIAL implementation

The serial implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_SERIAL, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, and a boolean flag *own_data* which specifies the ownership of *data*.

```
struct _N_VectorContent_Serial {
  sunindextype length;
  booleantype own_data;
  realtype *data;
};
```

The header file to be included when using this module is `nvector_serial.h`.

The following five macros are provided to access the content of an NVECTOR_SERIAL vector. The suffix `_S` in the names denotes the serial version.

- `NV_CONTENT_S`

  This routine gives access to the contents of the serial vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_S(v)` sets `v_cont` to be a pointer to the serial `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
  ```

- `NV_OWN_DATA_S`, `NV_DATA_S`, `NV_LENGTH_S`

  These macros give individual access to the parts of the content of a serial `N_Vector`.

  The assignment `v_data = NV_DATA_S(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_S(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

The assignment `v_len = NV_LENGTH_S(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_S(v) = len_v` sets the length of `v` to be `len_v`.

Implementation:

```
#define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )
#define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )
#define NV_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
```

- `NV_Ith_S`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_S(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_S(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_S(v,i) ( NV_DATA_S(v)[i] )
  ```

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Serial` (e.g. `N_VDestroy_Serial`). The module NVECTOR_SERIAL provides the following additional user-callable routines:

- `N_VNew_Serial`

  This function creates and allocates memory for a serial `N_Vector`. Its only argument is the vector length.

  ```
  N_Vector N_VNew_Serial(sunindextype vec_length);
  ```

- `N_VNewEmpty_Serial`

  This function creates a new serial `N_Vector` with an empty (`NULL`) data array.

  ```
  N_Vector N_VNewEmpty_Serial(sunindextype vec_length);
  ```

- `N_VMake_Serial`

  This function creates and allocates memory for a serial vector with user-provided data array.

  (This function does *not* allocate memory for `v_data` itself.)

  ```
  N_Vector N_VMake_Serial(sunindextype vec_length, realtype *v_data);
  ```

- `N_VCloneVectorArray_Serial`

  This function creates (by cloning) an array of `count` serial vectors.

  ```
  N_Vector *N_VCloneVectorArray_Serial(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Serial`

  This function creates (by cloning) an array of `count` serial vectors, each with an empty (`NULL`) data array.

  ```
  N_Vector *N_VCloneVectorArrayEmpty_Serial(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_Serial`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Serial` or with `N_VCloneVectorArrayEmpty_Serial`.

  ```
  void N_VDestroyVectorArray_Serial(N_Vector *vs, int count);
  ```

- `N_VGetLength_Serial`

  This function returns the number of vector elements.

  ```
  sunindextype N_VGetLength_Serial(N_Vector v);
  ```

- N_VPrint_Serial

  This function prints the content of a serial vector to stdout.

  ```
  void N_VPrint_Serial(N_Vector v);
  ```

Notes

- When looping over the components of an N_Vector v, it is more efficient to first obtain the component array via v_data = NV_DATA_S(v) and then access v_data[i] within the loop than it is to use NV_Ith_S(v,i) within the loop.

- N_VNewEmpty_Serial, N_VMake_Serial, and N_VCloneVectorArrayEmpty_Serial set the field *own_data* = FALSE. N_VDestroy_Serial and N_VDestroyVectorArray_Serial will not attempt to free the pointer *data* for any N_Vector with *own_data* set to FALSE. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_SERIAL implementation that have more than one N_Vector argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with N_Vector arguments that were all created with the same internal representations.

For solvers that include a Fortran interface module, the NVECTOR_SERIAL module also includes a Fortran-callable function FNVINITS(code, NEQ, IER), to initialize this NVECTOR_SERIAL module. Here code is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type long int); and IER is an error return flag equal 0 for success and -1 for failure.

7.2 The NVECTOR_PARALLEL implementation

The NVECTOR_PARALLEL implementation of the NVECTOR module provided with SUNDIALS is based on MPI. It defines the *content* field of N_Vector to be a structure containing the global and local lengths of the vector, a pointer to the beginning of a contiguous local data array, an MPI communicator, and a boolean flag *own_data* indicating ownership of the data array *data*.

```
struct _N_VectorContent_Parallel {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_data;
  realtype *data;
  MPI_Comm comm;
};
```

The header file to be included when using this module is nvector_parallel.h.

The following seven macros are provided to access the content of a NVECTOR_PARALLEL vector. The suffix _P in the names denotes the distributed memory parallel version.

- NV_CONTENT_P

  This macro gives access to the contents of the parallel vector N_Vector.

  The assignment v_cont = NV_CONTENT_P(v) sets v_cont to be a pointer to the N_Vector content structure of type struct _N_VectorContent_Parallel.

  Implementation:

  ```
  #define NV_CONTENT_P(v) ( (N_VectorContent_Parallel)(v->content) )
  ```

- NV_OWN_DATA_P, NV_DATA_P, NV_LOCLENGTH_P, NV_GLOBLENGTH_P

  These macros give individual access to the parts of the content of a parallel N_Vector.

  The assignment v_data = NV_DATA_P(v) sets v_data to be a pointer to the first component of the local data for the N_Vector v. The assignment NV_DATA_P(v) = v_data sets the component array of v to be v_data by storing the pointer v_data.

  The assignment v_llen = NV_LOCLENGTH_P(v) sets v_llen to be the length of the local part of v. The call NV_LENGTH_P(v) = llen_v sets the local length of v to be llen_v.

  The assignment v_glen = NV_GLOBLENGTH_P(v) sets v_glen to be the global length of the vector v. The call NV_GLOBLENGTH_P(v) = glen_v sets the global length of v to be glen_v.

  Implementation:

```
#define NV_OWN_DATA_P(v)    ( NV_CONTENT_P(v)->own_data )
#define NV_DATA_P(v)        ( NV_CONTENT_P(v)->data )
#define NV_LOCLENGTH_P(v)   ( NV_CONTENT_P(v)->local_length )
#define NV_GLOBLENGTH_P(v) ( NV_CONTENT_P(v)->global_length )
```

- NV_COMM_P

  This macro provides access to the MPI communicator used by the NVECTOR_PARALLEL vectors.

  Implementation:

```
#define NV_COMM_P(v) ( NV_CONTENT_P(v)->comm )
```

- NV_Ith_P

  This macro gives access to the individual components of the local data array of an N_Vector.

  The assignment r = NV_Ith_P(v,i) sets r to be the value of the i-th component of the local part of v. The assignment NV_Ith_P(v,i) = r sets the value of the i-th component of the local part of v to be r.

  Here i ranges from 0 to $n-1$, where n is the local length.

  Implementation:

```
#define NV_Ith_P(v,i) ( NV_DATA_P(v)[i] )
```

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Table 7.2 Their names are obtained from those in Table 7.2 by appending the suffix _Parallel (e.g. N_VDestroy_Parallel). The module NVECTOR_PARALLEL provides the following additional user-callable routines:

- N_VNew_Parallel

  This function creates and allocates memory for a parallel vector.

```
N_Vector N_VNew_Parallel(MPI_Comm comm,
                         sunindextype local_length,
                         sunindextype global_length);
```

- N_VNewEmpty_Parallel

  This function creates a new parallel N_Vector with an empty (NULL) data array.

```
N_Vector N_VNewEmpty_Parallel(MPI_Comm comm,
                              sunindextype local_length,
                              sunindextype global_length);
```

- N_VMake_Parallel

  This function creates and allocates memory for a parallel vector with user-provided data array. (This function does *not* allocate memory for v_data itself.)

```
N_Vector N_VMake_Parallel(MPI_Comm comm,
                          sunindextype local_length,
                          sunindextype global_length,
                          realtype *v_data);
```

- N_VCloneVectorArray_Parallel

  This function creates (by cloning) an array of count parallel vectors.

```
N_Vector *N_VCloneVectorArray_Parallel(int count, N_Vector w);
```

- N_VCloneVectorArrayEmpty_Parallel

  This function creates (by cloning) an array of count parallel vectors, each with an empty (NULL) data array.

```
N_Vector *N_VCloneVectorArrayEmpty_Parallel(int count, N_Vector w);
```

- N_VDestroyVectorArray_Parallel

  This function frees memory allocated for the array of count variables of type N_Vector created with N_VCloneVectorArray_Parallel or with N_VCloneVectorArrayEmpty_Parallel.

```
void N_VDestroyVectorArray_Parallel(N_Vector *vs, int count);
```

- N_VGetLength_Parallel

  This function returns the number of vector elements (global vector length).

```
sunindextype N_VGetLength_Parallel(N_Vector v);
```

- N_VGetLocalLength_Parallel

  This function returns the local vector length.

```
sunindextype N_VGetLocalLength_Parallel(N_Vector v);
```

- N_VPrint_Parallel

  This function prints the content of a parallel vector to stdout.

```
void N_VPrint_Parallel(N_Vector v);
```

Notes

- When looping over the components of an N_Vector v, it is more efficient to first obtain the local component array via v_data = NV_DATA_P(v) and then access v_data[i] within the loop than it is to use NV_Ith_P(v,i) within the loop.

- N_VNewEmpty_Parallel, N_VMake_Parallel, and N_VCloneVectorArrayEmpty_Parallel set the field *own_data* = FALSE. N_VDestroy_Parallel and N_VDestroyVectorArray_Parallel will not attempt to free the pointer *data* for any N_Vector with *own_data* set to FALSE. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PARALLEL implementation that have more than one N_Vector argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with N_Vector arguments that were all created with the same internal representations.

For solvers that include a Fortran interface module, the NVECTOR_PARALLEL module also includes a Fortran-callable function `FNVINITP(COMM, code, NLOCAL, NGLOBAL, IER)`, to initialize this NVECTOR_PARALLEL module. Here `COMM` is the MPI communicator, `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `NLOCAL` and `NGLOBAL` are the local and global vector sizes, respectively (declared so as to match C type `long int`); and IER is an error return flag equal 0 for success and -1 for failure. NOTE: If the header file `sundials_config.h` defines `SUNDIALS_MPI_COMM_F2C` to be 1 (meaning the MPI implementation used to build SUNDIALS includes the `MPI_Comm_f2c` function), then `COMM` can be any valid MPI communicator. Otherwise, `MPI_COMM_WORLD` will be used, so just pass an integer value as a placeholder.

7.3 The NVECTOR_OPENMP implementation

In situations where a user has a multi-core processing unit capable of running multiple parallel threads with shared memory, SUNDIALS provides an implementation of NVECTOR using OpenMP, called NVECTOR_OPENMP, and an implementation using Pthreads, called NVECTOR_PTHREADS. Testing has shown that vectors should be of length at least 100,000 before the overhead associated with creating and using the threads is made up by the parallelism in the vector calculations.

The OpenMP NVECTOR implementation provided with SUNDIALS, NVECTOR_OPENMP, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, a boolean flag *own_data* which specifies the ownership of *data*, and the number of threads. Operations on the vector are threaded using OpenMP.

```
struct _N_VectorContent_OpenMP {
  sunindextype length;
  booleantype own_data;
  realtype *data;
  int num_threads;
};
```

The header file to be included when using this module is `nvector_openmp.h`.

The following six macros are provided to access the content of an NVECTOR_OPENMP vector. The suffix `_OMP` in the names denotes the OpenMP version.

- `NV_CONTENT_OMP`

  This routine gives access to the contents of the OpenMP vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_OMP(v)` sets `v_cont` to be a pointer to the OpenMP `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_OMP(v) ( (N_VectorContent_OpenMP)(v->content) )
  ```

- `NV_OWN_DATA_OMP`, `NV_DATA_OMP`, `NV_LENGTH_OMP`, `NV_NUM_THREADS_OMP`

  These macros give individual access to the parts of the content of a OpenMP `N_Vector`.

  The assignment `v_data = NV_DATA_OMP(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_OMP(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_len = NV_LENGTH_OMP(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_OMP(v) = len_v` sets the length of `v` to be `len_v`.

  The assignment `v_num_threads = NV_NUM_THREADS_OMP(v)` sets `v_num_threads` to be the number of threads from `v`. On the other hand, the call `NV_NUM_THREADS_OMP(v) = num_threads_v` sets the number of threads for `v` to be `num_threads_v`.

  Implementation:

  ```
  #define NV_OWN_DATA_OMP(v) ( NV_CONTENT_OMP(v)->own_data )
  ```

```
#define NV_DATA_OMP(v) ( NV_CONTENT_OMP(v)->data )
#define NV_LENGTH_OMP(v) ( NV_CONTENT_OMP(v)->length )
#define NV_NUM_THREADS_OMP(v) ( NV_CONTENT_OMP(v)->num_threads )
```

- `NV_Ith_OMP`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_OMP(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_OMP(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_OMP(v,i) ( NV_DATA_OMP(v)[i] )
  ```

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_OpenMP` (e.g. `N_VDestroy_OpenMP`). The module NVECTOR_OPENMP provides the following additional user-callable routines:

- `N_VNew_OpenMP`

  This function creates and allocates memory for a OpenMP `N_Vector`. Arguments are the vector length and number of threads.

  ```
  N_Vector N_VNew_OpenMP(sunindextype vec_length, int num_threads);
  ```

- `N_VNewEmpty_OpenMP`

  This function creates a new OpenMP `N_Vector` with an empty (`NULL`) data array.

  ```
  N_Vector N_VNewEmpty_OpenMP(sunindextype vec_length, int num_threads);
  ```

- `N_VMake_OpenMP`

  This function creates and allocates memory for a OpenMP vector with user-provided data array.

  (This function does *not* allocate memory for `v_data` itself.)

  ```
  N_Vector N_VMake_OpenMP(sunindextype vec_length, realtype *v_data, int num_threads);
  ```

- `N_VCloneVectorArray_OpenMP`

  This function creates (by cloning) an array of `count` OpenMP vectors.

  ```
  N_Vector *N_VCloneVectorArray_OpenMP(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_OpenMP`

  This function creates (by cloning) an array of `count` OpenMP vectors, each with an empty (`NULL`) data array.

  ```
  N_Vector *N_VCloneVectorArrayEmpty_OpenMP(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_OpenMP`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_OpenMP` or with `N_VCloneVectorArrayEmpty_OpenMP`.

  ```
  void N_VDestroyVectorArray_OpenMP(N_Vector *vs, int count);
  ```

- `N_VGetLength_OpenMP`

  This function returns number of vector elements.

  ```
  sunindextype N_VGetLength_OpenMP(N_Vector v);
  ```

- `N_VPrint_OpenMP`

  This function prints the content of a OpenMP vector to `stdout`.

  ```
  void N_VPrint_OpenMP(N_Vector v);
  ```

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_OMP(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_OMP(v,i)` within the loop.

- `N_VNewEmpty_OpenMP`, `N_VMake_OpenMP`, and `N_VCloneVectorArrayEmpty_OpenMP` set the field *own_data* = `FALSE`. `N_VDestroy_OpenMP` and `N_VDestroyVectorArray_OpenMP` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `FALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_OPENMP implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

For solvers that include a Fortran interface module, the NVECTOR_OPENMP module also includes a Fortran-callable function `FNVINITOMP(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type `long int`); NUMTHREADS is the number of threads; and IER is an error return flag equal 0 for success and -1 for failure.

7.4 The NVECTOR_PTHREADS implementation

In situations where a user has a multi-core processing unit capable of running multiple parallel threads with shared memory, SUNDIALS provides an implementation of NVECTOR using OpenMP, called NVECTOR_OPENMP, and an implementation using Pthreads, called NVECTOR_PTHREADS. Testing has shown that vectors should be of length at least 100,000 before the overhead associated with creating and using the threads is made up by the parallelism in the vector calculations.

The Pthreads NVECTOR implementation provided with SUNDIALS, denoted NVECTOR_PTHREADS, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, a boolean flag *own_data* which specifies the ownership of *data*, and the number of threads. Operations on the vector are threaded using POSIX threads (Pthreads).

```
struct _N_VectorContent_Pthreads {
  sunindextype length;
  booleantype own_data;
  realtype *data;
  int num_threads;
};
```

The header file to be included when using this module is `nvector_pthreads.h`.

The following six macros are provided to access the content of an NVECTOR_PTHREADS vector. The suffix `_PT` in the names denotes the Pthreads version.

- `NV_CONTENT_PT`

  This routine gives access to the contents of the Pthreads vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_PT(v)` sets `v_cont` to be a pointer to the Pthreads `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_PT(v) ( (N_VectorContent_Pthreads)(v->content) )
  ```

- `NV_OWN_DATA_PT`, `NV_DATA_PT`, `NV_LENGTH_PT`, `NV_NUM_THREADS_PT`

  These macros give individual access to the parts of the content of a Pthreads `N_Vector`.

The assignment `v_data = NV_DATA_PT(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_PT(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

The assignment `v_len = NV_LENGTH_PT(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_PT(v) = len_v` sets the length of `v` to be `len_v`.

The assignment `v_num_threads = NV_NUM_THREADS_PT(v)` sets `v_num_threads` to be the number of threads from `v`. On the other hand, the call `NV_NUM_THREADS_PT(v) = num_threads_v` sets the number of threads for `v` to be `num_threads_v`.

Implementation:

```
#define NV_OWN_DATA_PT(v) ( NV_CONTENT_PT(v)->own_data )
#define NV_DATA_PT(v) ( NV_CONTENT_PT(v)->data )
#define NV_LENGTH_PT(v) ( NV_CONTENT_PT(v)->length )
#define NV_NUM_THREADS_PT(v) ( NV_CONTENT_PT(v)->num_threads )
```

- `NV_Ith_PT`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_PT(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_PT(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_PT(v,i) ( NV_DATA_PT(v)[i] )
  ```

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Pthreads` (e.g. `N_VDestroy_Pthreads`). The module NVECTOR_PTHREADS provides the following additional user-callable routines:

- `N_VNew_Pthreads`

  This function creates and allocates memory for a Pthreads `N_Vector`. Arguments are the vector length and number of threads.

  ```
  N_Vector N_VNew_Pthreads(sunindextype vec_length, int num_threads);
  ```

- `N_VNewEmpty_Pthreads`

  This function creates a new Pthreads `N_Vector` with an empty (`NULL`) data array.

  ```
  N_Vector N_VNewEmpty_Pthreads(sunindextype vec_length, int num_threads);
  ```

- `N_VMake_Pthreads`

  This function creates and allocates memory for a Pthreads vector with user-provided data array.

  (This function does *not* allocate memory for `v_data` itself.)

  ```
  N_Vector N_VMake_Pthreads(sunindextype vec_length, realtype *v_data, int num_threads);
  ```

- `N_VCloneVectorArray_Pthreads`

  This function creates (by cloning) an array of `count` Pthreads vectors.

  ```
  N_Vector *N_VCloneVectorArray_Pthreads(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Pthreads`

  This function creates (by cloning) an array of `count` Pthreads vectors, each with an empty (`NULL`) data array.

  ```
  N_Vector *N_VCloneVectorArrayEmpty_Pthreads(int count, N_Vector w);
  ```

- N_VDestroyVectorArray_Pthreads

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Pthreads` or with `N_VCloneVectorArrayEmpty_Pthreads`.

  ```
  void N_VDestroyVectorArray_Pthreads(N_Vector *vs, int count);
  ```

- N_VGetLength_Pthreads

  This function returns the number of vector elements.

  ```
  sunindextype N_VGetLength_Pthreads(N_Vector v);
  ```

- N_VPrint_Pthreads

  This function prints the content of a Pthreads vector to `stdout`.

  ```
  void N_VPrint_Pthreads(N_Vector v);
  ```

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_PT(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_PT(v,i)` within the loop.

- `N_VNewEmpty_Pthreads`, `N_VMake_Pthreads`, and `N_VCloneVectorArrayEmpty_Pthreads` set the field *own_data* = `FALSE`. `N_VDestroy_Pthreads` and `N_VDestroyVectorArray_Pthreads` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `FALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PTHREADS implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

For solvers that include a Fortran interface module, the NVECTOR_PTHREADS module also includes a Fortran-callable function `FNVINITPTS(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type `long int`); NUMTHREADS is the number of threads; and IER is an error return flag equal 0 for success and -1 for failure.

7.5 The NVECTOR_PARHYP implementation

The NVECTOR_PARHYP implementation of the NVECTOR module provided with SUNDIALS is a wrapper around *hypre*'s ParVector class. Most of the vector kernels simply call *hypre* vector operations. The implementation defines the *content* field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to an object of type `hypre_ParVector`, an MPI communicator, and a boolean flag *own_parvector* indicating ownership of the *hypre* parallel vector object x.

```
struct _N_VectorContent_ParHyp {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_parvector;
  MPI_Comm comm;
  hypre_ParVector *x;
};
```

The header file to be included when using this module is `nvector_parhyp.h`. Unlike native SUNDIALS vector types, NVECTOR_PARHYP does not provide macros to access its member variables.

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Table 7.2, except for `N_VSetArrayPointer` and `N_VGetArrayPointer`, because accessing raw vector data is

handled by low-level *hypre* functions. As such, this vector is not available for use with SUNDIALS Fortran interfaces. When access to raw vector data is needed, one should extract *hypre* vector first, and then use *hypre* methods to access the data. Usage examples of NVECTOR_PARHYP are provided in the `cvAdvDiff_non_ph.c` example program for CVODE [25] and the `ark_diurnal_kry_ph.c` example program for ARKODE [31].

The names of parhyp methods are obtained from those in Table 7.2 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR_PARHYP provides the following additional user-callable routines:

- `N_VNewEmpty_ParHyp`

  This function creates a new parhyp `N_Vector` with the pointer to the *hypre* vector set to `NULL`.

  ```
  N_Vector N_VNewEmpty_ParHyp(MPI_Comm comm,
                              sunindextype local_length,
                              sunindextype global_length);
  ```

- `N_VMake_ParHyp`

  This function creates an `N_Vector` wrapper around an existing *hypre* parallel vector. It does *not* allocate memory for `x` itself.

  ```
  N_Vector N_VMake_ParHyp(hypre_ParVector *x);
  ```

- `N_VGetVector_ParHyp`

  This function returns a pointer to the underlying *hypre* vector.

  ```
  hypre_ParVector *N_VGetVector_ParHyp(N_Vector v);
  ```

- `N_VCloneVectorArray_ParHyp`

  This function creates (by cloning) an array of `count` parallel vectors.

  ```
  N_Vector *N_VCloneVectorArray_ParHyp(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_ParHyp`

  This function creates (by cloning) an array of `count` parallel vectors, each with an empty (`NULL`) data array.

  ```
  N_Vector *N_VCloneVectorArrayEmpty_ParHyp(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_ParHyp`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_ParHyp` or with `N_VCloneVectorArrayEmpty_ParHyp`.

  ```
  void N_VDestroyVectorArray_ParHyp(N_Vector *vs, int count);
  ```

- `N_VPrint_ParHyp`

  This function prints the content of a parhyp vector to stdout.

  ```
  void N_VPrint_ParHyp(N_Vector v);
  ```

Notes

- When there is a need to access components of an `N_Vector_ParHyp`, `v`, it is recommended to extract the *hypre* vector via `x_vec = N_VGetVector_ParHyp(v)` and then access components using appropriate *hypre* functions.

- `N_VNewEmpty_ParHyp`, `N_VMake_ParHyp`, and `N_VCloneVectorArrayEmpty_ParHyp` set the field *own_parvector* to `FALSE`. `N_VDestroy_ParHyp` and `N_VDestroyVectorArray_ParHyp` will not attempt to delete an underlying *hypre* vector for any `N_Vector` with *own_parvector* set to `FALSE`. In such a case, it is the user's responsibility to delete the underlying vector.

- To maximize efficiency, vector operations in the NVECTOR_PARHYP implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.6 The NVECTOR_PETSC implementation

The NVECTOR_PETSC module is an NVECTOR wrapper around the PETSc vector. It defines the *content* field of a `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the PETSc vector, an MPI communicator, and a boolean flag *own_data* indicating ownership of the wrapped PETSc vector.

```
struct _N_VectorContent_Petsc {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_data;
  Vec *pvec;
  MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_petsc.h`. Unlike native SUNDIALS vector types, NVECTOR_PETSC does not provide macros to access its member variables. Note that NVECTOR_PETSC requires SUNDIALS to be built with MPI support.

The NVECTOR_PETSC module defines implementations of all vector operations listed in Table 7.2, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with SUNDIALS Fortran interfaces. When access to raw vector data is needed, it is recommended to extract the PETSc vector first, and then use PETSc methods to access the data. Usage examples of NVECTOR_PETSC are provided in example programs for IDA [23].

The names of vector operations are obtained from those in Table 7.2 by appending the suffix `_Petsc` (e.g. `N_VDestroy_Petsc`). The module NVECTOR_PETSC provides the following additional user-callable routines:

- `N_VNewEmpty_Petsc`

  This function creates a new NVECTOR wrapper with the pointer to the wrapped PETSc vector set to (`NULL`). It is used by the `N_VMake_Petsc` and `N_VClone_Petsc` implementations.

  ```
  N_Vector N_VNewEmpty_Petsc(MPI_Comm comm,
                             sunindextype local_length,
                             sunindextype global_length);
  ```

- `N_VMake_Petsc`

  This function creates and allocates memory for an NVECTOR_PETSC wrapper around a user-provided PETSc vector. It does *not* allocate memory for the vector `pvec` itself.

```
N_Vector N_VMake_Petsc(Vec *pvec);
```

- `N_VGetVector_Petsc`

  This function returns a pointer to the underlying PETSc vector.

  ```
  Vec *N_VGetVector_Petsc(N_Vector v);
  ```

- `N_VCloneVectorArray_Petsc`

  This function creates (by cloning) an array of `count` NVECTOR_PETSC vectors.

  ```
  N_Vector *N_VCloneVectorArray_Petsc(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Petsc`

  This function creates (by cloning) an array of `count` NVECTOR_PETSC vectors, each with pointers to PETSc vectors set to (`NULL`).

  ```
  N_Vector *N_VCloneEmptyVectorArray_Petsc(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_Petsc`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Petsc` or with `N_VCloneVectorArrayEmpty_Petsc`.

  ```
  void N_VDestroyVectorArray_Petsc(N_Vector *vs, int count);
  ```

- `N_VPrint_Petsc`

  This function prints the content of a wrapped PETSc vector to stdout.

  ```
  void N_VPrint_Petsc(N_Vector v);
  ```

Notes

- When there is a need to access components of an `N_Vector_Petsc`, `v`, it is recommeded to extract the PETSc vector via `x_vec = N_VGetVector_Petsc(v)` and then access components using appropriate PETSc functions.

- The functions `N_VNewEmpty_Petsc`, `N_VMake_Petsc`, and `N_VCloneVectorArrayEmpty_Petsc` set the field *own_data* to `FALSE`. `N_VDestroy_Petsc` and `N_VDestroyVectorArray_Petsc` will not attempt to free the pointer *pvec* for any `N_Vector` with *own_data* set to `FALSE`. In such a case, it is the user's responsibility to deallocate the *pvec* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PETSC implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.7 The NVECTOR_CUDA implementation

The NVECTOR_CUDA module is an experimental implementation of NVECTOR in the CUDA language. The module allows for SUNDIALS vector kernels to run on GPU devices. It is intended for users who are already familiar with CUDA and GPU programming. Building this vector module requires a CUDA compiler and, by extension, a C++ compiler. The class `Vector` in namespace `suncudavec` manages vector data layout:

```
template <class T, class I>
class Vector {
  I size_;
  I mem_size_;
  T* h_vec_;
  T* d_vec_;
  StreamPartitioning<T, I>* partStream_;
  ReducePartitioning<T, I>* partReduce_;
  bool ownPartitioning_;

  ...
};
```

The class members are vector size (length), size of the vector data memory block, pointers to vector data on the host and the device, pointers to classes `StreamPartitioning` and `ReducePartitioning`, which handle thread partitioning for streaming and reduction vector kernels, respectively, and a boolean flag that signals if the vector owns the thread partitioning. The class `Vector` inherits from the empty structure

```
struct _N_VectorContent_Cuda {
};
```

to interface the C++ class with the NVECTOR C code. When instantiated, the class `Vector` will allocate memory on both the host and the device. Due to the rapid progress of CUDA development, we expect that the `suncudavec::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `suncudavec::Vector` class without requiring changes to the user API.

The header file to be included when using this module is `nvector_cuda.h`. Unlike other native SUNDIALS vector types, NVECTOR_CUDA does not provide macros to access its member variables. Note that NVECTOR_CUDA requires SUNDIALS to be built with MPI support.

The NVECTOR_CUDA module defines implementations of all vector operations listed in Table 7.2, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor with SUNDIALS direct solvers and preconditioners. This support will be added in subsequent SUNDIALS releases. The NVECTOR_CUDA module provides separate functions to access data on the host and on the device. It also provides methods for copying from the host to the device and vice versa. Usage examples of NVECTOR_CUDA are provided in some example programs for CVODE [25].

The names of vector operations are obtained from those in Table 7.2 by appending the suffix `_Cuda` (e.g. `N_VDestroy_Cuda`). The module NVECTOR_CUDA provides the following additional user-callable routines:

- `N_VNew_Cuda`

  This function creates and allocates memory for a CUDA `N_Vector`. The memory is allocated on both host and device. Its only argument is the vector length.

  ```
  N_Vector N_VNew_Cuda(sunindextype vec_length);
  ```

- `N_VNewEmpty_Cuda`

  This function creates a new NVECTOR wrapper with the pointer to the wrapped CUDA vector set to (`NULL`). It is used by the `N_VNew_Cuda`, `N_VMake_Cuda`, and `N_VClone_Cuda` implementations.

  ```
  N_Vector N_VNewEmpty_Cuda(sunindextype vec_length);
  ```

- `N_VMake_Cuda`

This function creates and allocates memory for an NVECTOR_CUDA wrapper around a user-provided `suncudavec::Vector` class. Its only argument is of type `N_VectorContent_Cuda`, which is the pointer to the class.

```
N_Vector N_VMake_Cuda(N_VectorContent_Cuda c);
```

- `N_VCloneVectorArray_Cuda`

  This function creates (by cloning) an array of `count` NVECTOR_CUDA vectors.

  ```
  N_Vector *N_VCloneVectorArray_Cuda(int count, N_Vector w);
  ```

- `N_VCloneVectorArrayEmpty_Cuda`

  This function creates (by cloning) an array of `count` NVECTOR_CUDA vectors, each with pointers to CUDA vectors set to (`NULL`).

  ```
  N_Vector *N_VCloneEmptyVectorArray_Cuda(int count, N_Vector w);
  ```

- `N_VDestroyVectorArray_Cuda`

  This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Cuda` or with `N_VCloneVectorArrayEmpty_Cuda`.

  ```
  void N_VDestroyVectorArray_Cuda(N_Vector *vs, int count);
  ```

- `N_VGetLength_Cuda`

  This function returns the length of the vector.

  ```
  sunindextype N_VGetLength_Cuda(N_Vector v);
  ```

- `N_VGetHostArrayPointer_Cuda`

  This function returns a pointer to the vector data on the host.

  ```
  realtype *N_VGetHostArrayPointer_Cuda(N_Vector v);
  ```

- `N_VGetDeviceArrayPointer_Cuda`

  This function returns a pointer to the vector data on the device.

  ```
  realtype *N_VGetDeviceArrayPointer_Cuda(N_Vector v);
  ```

- `N_VCopyToDevice_Cuda`

  This function copies host vector data to the device.

  ```
  realtype *N_VCopyToDevice_Cuda(N_Vector v);
  ```

- `N_VCopyFromDevice_Cuda`

  This function copies vector data from the device to the host.

  ```
  realtype *N_VCopyFromDevice_Cuda(N_Vector v);
  ```

- `N_VPrint_Cuda`

  This function prints the content of a wrapped CUDA vector to stdout.

  ```
  void N_VPrint_Cuda(N_Vector v);
  ```

Notes

- When there is a need to access components of an `N_Vector_Cuda`, `v`, it is recommeded to use functions `N_VGetDeviceArrayPointer_Cuda` or `N_VGetHostArrayPointer_Cuda`.
- To maximize efficiency, vector operations in the NVECTOR_CUDA implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.8 The NVECTOR_RAJA implementation

The NVECTOR_RAJA module is an experimental implementation of NVECTOR using the RAJA hardware abstraction layer, https://software.llnl.gov/RAJA/. In this implementation, RAJA allows for SUNDIALS vector kernels to run on GPU devices. The module is intended for users who are already familiar with RAJA and GPU programming. Building this vector module requires a C++11 compliant compiler and a CUDA software development toolkit. Besides the CUDA backend, RAJA has other backends such as serial, OpenMP, and OpenAC. These backends are not used in this SUNDIALS release. Class `Vector` in namespace `sunrajavec` manages the vector data layout:

```
template <class T, class I>
class Vector {
  I size_;
  I mem_size_;
  T* h_vec_;
  T* d_vec_;

  ...
};
```

The class members are: vector size (length), size of the vector data memory block, and pointers to vector data on the host and on the device. The class `Vector` inherits from an empty structure

```
struct _N_VectorContent_Raja {
};
```

to interface the C++ class with the NVECTOR C code. When instantiated, the class `Vector` will allocate memory on both the host and the device. Due to the rapid progress of RAJA development, we expect that the `sunrajavec::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `sunrajavec::Vector` class without requiring changes to the user API.

The header file to be included when using this module is `nvector_raja.h`. Unlike other native SUNDIALS vector types, NVECTOR_RAJA does not provide macros to access its member variables. Note that NVECTOR_RAJA requires SUNDIALS to be built with MPI support.

The NVECTOR_RAJA module defines the implementations of all vector operations listed in Table 7.2, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor with SUNDIALS direct solvers and preconditioners. The NVECTOR_RAJA module provides separate functions to access data on the host and on the device. It also provides methods for copying data from the host to the device and vice versa. Usage examples of NVECTOR_RAJA are provided in some example programs for CVODE [25].

The names of vector operations are obtained from those in Table 7.2 by appending the suffix `_Raja` (e.g. `N_VDestroy_Raja`). The module NVECTOR_RAJA provides the following additional user-callable routines:

- `N_VNew_Raja`

  This function creates and allocates memory for a RAJA `N_Vector`. The memory is allocated on both the host and the device. Its only argument is the vector length.

```
N_Vector N_VNew_Raja(sunindextype vec_length);
```

- N_VNewEmpty_Raja

  This function creates a new NVECTOR wrapper with the pointer to the wrapped RAJA vector set to (NULL). It is used by the N_VNew_Raja, N_VMake_Raja, and N_VClone_Raja implementations.

  ```
  N_Vector N_VNewEmpty_Raja(sunindextype vec_length);
  ```

- N_VMake_Raja

  This function creates and allocates memory for an NVECTOR_RAJA wrapper around a user-provided sunrajavec::Vector class. Its only argument is of type N_VectorContent_Raja, which is the pointer to the class.

  ```
  N_Vector N_VMake_Raja(N_VectorContent_Raja c);
  ```

- N_VCloneVectorArray_Raja

  This function creates (by cloning) an array of count NVECTOR_RAJA vectors.

  ```
  N_Vector *N_VCloneVectorArray_Raja(int count, N_Vector w);
  ```

- N_VCloneVectorArrayEmpty_Raja

  This function creates (by cloning) an array of count NVECTOR_RAJA vectors, each with pointers to RAJA vectors set to (NULL).

  ```
  N_Vector *N_VCloneEmptyVectorArray_Raja(int count, N_Vector w);
  ```

- N_VDestroyVectorArray_Raja

  This function frees memory allocated for the array of count variables of type N_Vector created with N_VCloneVectorArray_Raja or with N_VCloneVectorArrayEmpty_Raja.

  ```
  void N_VDestroyVectorArray_Raja(N_Vector *vs, int count);
  ```

- N_VGetLength_Raja

  This function returns the length of the vector.

  ```
  sunindextype N_VGetLength_Raja(N_Vector v);
  ```

- N_VGetHostArrayPointer_Raja

  This function returns a pointer to the vector data on the host.

  ```
  realtype *N_VGetHostArrayPointer_Raja(N_Vector v);
  ```

- N_VGetDeviceArrayPointer_Raja

  This function returns a pointer to the vector data on the device.

  ```
  realtype *N_VGetDeviceArrayPointer_Raja(N_Vector v);
  ```

- N_VCopyToDevice_Raja

  This function copies host vector data to the device.

  ```
  realtype *N_VCopyToDevice_Raja(N_Vector v);
  ```

- N_VCopyFromDevice_Raja

  This function copies vector data from the device to the host.

  ```
  realtype *N_VCopyFromDevice_Raja(N_Vector v);
  ```

- N_VPrint_Raja

  This function prints the content of a wrapped RAJA vector to stdout.

  ```
  void N_VPrint_Raja(N_Vector v);
  ```

Notes

- When there is a need to access components of an `N_Vector_Raja`, `v`, it is recommeded to use functions `N_VGetDeviceArrayPointer_Raja` or `N_VGetHostArrayPointer_Raja`.
- To maximize efficiency, vector operations in the NVECTOR_RAJA implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.9 NVECTOR Examples

There are `NVector` examples that may be installed for each implementation: serial, parallel, OpenMP, and Pthreads. Each implementation makes use of the functions in `test_nvector.c`. These example functions show simple usage of the `NVector` family of functions. The input to the examples are the vector length, number of threads (if threaded implementation), and a print timing flag.
The following is a list of the example functions in `test_nvector.c`:

- `Test_N_VClone`: Creates clone of vector and checks validity of clone.
- `Test_N_VCloneEmpty`: Creates clone of empty vector and checks validity of clone.
- `Test_N_VCloneVectorArray`: Creates clone of vector array and checks validity of cloned array.
- `Test_N_VCloneVectorArray`: Creates clone of empty vector array and checks validity of cloned array.
- `Test_N_VGetArrayPointer`: Get array pointer.
- `Test_N_VSetArrayPointer`: Allocate new vector, set pointer to new vector array, and check values.
- `Test_N_VLinearSum` Case 1a: Test y = x + y
- `Test_N_VLinearSum` Case 1b: Test y = -x + y
- `Test_N_VLinearSum` Case 1c: Test y = ax + y
- `Test_N_VLinearSum` Case 2a: Test x = x + y
- `Test_N_VLinearSum` Case 2b: Test x = x - y
- `Test_N_VLinearSum` Case 2c: Test x = x + by
- `Test_N_VLinearSum` Case 3: Test z = x + y
- `Test_N_VLinearSum` Case 4a: Test z = x - y
- `Test_N_VLinearSum` Case 4b: Test z = -x + y
- `Test_N_VLinearSum` Case 5a: Test z = x + by
- `Test_N_VLinearSum` Case 5b: Test z = ax + y
- `Test_N_VLinearSum` Case 6a: Test z = -x + by
- `Test_N_VLinearSum` Case 6b: Test z = ax - y
- `Test_N_VLinearSum` Case 7: Test z = a(x + y)
- `Test_N_VLinearSum` Case 8: Test z = a(x - y)

- `Test_N_VLinearSum` Case 9: Test z = ax + by
- `Test_N_VConst`: Fill vector with constant and check result.
- `Test_N_VProd`: Test vector multiply: z = x * y
- `Test_N_VDiv`: Test vector division: z = x / y
- `Test_N_VScale`: Case 1: scale: x = cx
- `Test_N_VScale`: Case 2: copy: z = x
- `Test_N_VScale`: Case 3: negate: z = -x
- `Test_N_VScale`: Case 4: combination: z = cx
- `Test_N_VAbs`: Create absolute value of vector.
- `Test_N_VAddConst`: add constant vector: z = c + x
- `Test_N_VDotProd`: Calculate dot product of two vectors.
- `Test_N_VMaxNorm`: Create vector with known values, find and validate max norm.
- `Test_N_VWrmsNorm`: Create vector of known values, find and validate weighted root mean square.
- `Test_N_VWrmsNormMask`: Case 1: Create vector of known values, find and validate weighted root mean square using all elements.
- `Test_N_VWrmsNormMask`: Case 2: Create vector of known values, find and validate weighted root mean square using no elements.
- `Test_N_VMin`: Create vector, find and validate the min.
- `Test_N_VWL2Norm`: Create vector, find and validate the weighted Euclidean L2 norm.
- `Test_N_VL1Norm`: Create vector, find and validate the L1 norm.
- `Test_N_VCompare`: Compare vector with constant returning and validating comparison vector.
- `Test_N_VInvTest`: Test z[i] = 1 / x[i]
- `Test_N_VConstrMask`: Test mask of vector x with vector c.
- `Test_N_VMinQuotient`: Fill two vectors with known values. Calculate and validate minimum quotient.

7.10 NVECTOR functions used by IDAS

In Table 7.3 below, we list the vector functions used in the NVECTOR module used by the IDAS package. The table also shows, for each function, which of the code modules uses the function. The IDAS column shows function usage within the main integrator module, while the remaining five columns show function usage within each of the five IDAS linear solvers, the IDABBDPRE preconditioner module, and the IDAS adjoint sensitivity module (denoted here by IDAA). Here IDADLS stands for IDADENSE and IDABAND; IDASPILS stands for IDASPGMR, IDASPBCG, and IDASPTFQMR; and IDASLS stands for IDAKLU and IDASUPERLUMT.

There is one subtlety in the IDASPILS column hidden by the table, explained here for the case of the IDASPGMR module. The `N_VDotProd` function is called both within the interface file `ida_spgmr.c` and within the implementation files `sundials_spgmr.c` and `sundials_iterative.c` for the generic SPGMR solver upon which the IDASPGMR solver is built. Also, although `N_VDiv` and `N_VProd` are not called within the interface file `ida_spgmr.c`, they are called within the implementation file

sundials_spgmr.c, and so are required by the IDASPGMR solver module. Analogous statements apply to the IDASPBCG and IDASPTFQMR modules, except that they do not use sundials_iterative.c. This issue does not arise for the direct IDAS linear solvers because the generic DENSE and BAND solvers (used in the implementation of IDADENSE and IDABAND) do not make calls to any vector functions.

Table 7.3: List of vector functions usage by IDAS code modules

	IDAS	IDADLS	IDASPILS	IDASLS	IDABBDPRE	IDAA
N_VGetVectorID						
N_VClone	✓		✓		✓	✓
N_VDestroy	✓		✓		✓	✓
N_VCloneVectorArray	✓					✓
N_VDestroyVectorArray	✓					✓
N_VSpace	✓					
N_VGetArrayPointer		✓		✓	✓	
N_VSetArrayPointer		✓				
N_VLinearSum	✓	✓	✓			✓
N_VConst	✓		✓			✓
N_VProd	✓		✓			
N_VDiv	✓		✓			
N_VScale	✓	✓	✓	✓	✓	✓
N_VAbs	✓					
N_VInv	✓					
N_VAddConst	✓					
N_VDotProd			✓			
N_VMaxNorm	✓					
N_VWrmsNorm	✓		✓			
N_VMin	✓					
N_VMinQuotient	✓					
N_VConstrMask	✓					
N_VWrmsNormMask	✓					
N_VCompare	✓					

Of the functions listed in Table 7.2, N_VWL2Norm, N_VL1Norm, N_VCloneEmpty, and N_VInvTest are *not* used by IDAS. Therefore a user-supplied NVECTOR module for IDAS could omit these four functions.

Chapter 8

Description of the SUNMatrix module

For problems that involve direct methods for solving linear systems, the SUNDIALS solvers not only operate on generic vectors, but also on generic matrices (of type `SUNMatrix`), through a set of operations defined by the particular SUNMATRIX implementation. Users can provide their own specific implementation of the SUNMATRIX module, particularly in cases where they provide their own NVECTOR and/or linear solver modules, and require matrices that are compatible with those implementations. Alternately, we provide three SUNMATRIX implementations: dense, banded, and sparse. The generic operations are described below, and descriptions of the implementations provided with SUNDIALS follow.

The generic `SUNMatrix` type has been modeled after the object-oriented style of the generic `N_Vector` type. Specifically, a generic `SUNMatrix` is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the matrix, and an *ops* field pointing to a structure with generic matrix operations. The type `SUNMatrix` is defined as

```
typedef struct _generic_SUNMatrix *SUNMatrix;

struct _generic_SUNMatrix {
    void *content;
    struct _generic_SUNMatrix_Ops *ops;
};
```

The `_generic_SUNMatrix_Ops` structure is essentially a list of pointers to the various actual matrix operations, and is defined as

```
struct _generic_SUNMatrix_Ops {
  SUNMatrix_ID (*getid)(SUNMatrix);
  SUNMatrix    (*clone)(SUNMatrix);
  void         (*destroy)(SUNMatrix);
  int          (*zero)(SUNMatrix);
  int          (*copy)(SUNMatrix, SUNMatrix);
  int          (*scaleadd)(realtype, SUNMatrix, SUNMatrix);
  int          (*scaleaddi)(realtype, SUNMatrix);
  int          (*matvec)(SUNMatrix, N_Vector, N_Vector);
  int          (*space)(SUNMatrix, long int*, long int*);
};
```

The generic SUNMATRIX module defines and implements the matrix operations acting on `SUNMatrix` objects. These routines are nothing but wrappers for the matrix operations defined by a particular SUNMATRIX implementation, which are accessed through the *ops* field of the `SUNMatrix` structure. To

Table 8.1: Identifiers associated with matrix kernels supplied with SUNDIALS.

Matrix ID	Matrix type	ID Value
SUNMATRIX_DENSE	Dense `M` $\times$ `N` matrix	0
SUNMATRIX_BAND	Band `M` $\times$ `M` matrix	1
SUNMATRIX_SPARSE	Sparse (CSR or CSC) `M` $\times$ `N` matrix	2
SUNMATRIX_CUSTOM	User-provided custom matrix	3

illustrate this point we show below the implementation of a typical matrix operation from the generic SUNMATRIX module, namely `SUNMatZero`, which sets all values of a matrix `A` to zero, returning a flag denoting a successful/failed operation:

```
int SUNMatZero(SUNMatrix A)
{
  return((int) A->ops->zero(A));
}
```

Table 8.2 contains a complete list of all matrix operations defined by the generic SUNMATRIX module. A particular implementation of the SUNMATRIX module must:

- Specify the *content* field of the `SUNMatrix` object.
- Define and implement a minimal subset of the matrix operations. See the documentation for each SUNDIALS solver to determine which SUNMATRIX operations they require.

  Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNMATRIX module (each with different `SUNMatrix` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free a `SUNMatrix` with the new *content* field and with *ops* pointing to the new matrix operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined `SUNMatrix` (e.g., a routine to print the content for debugging purposes).
- Optionally, provide accessor macros or functions as needed for that particular implementation to access different parts of the *content* field of the newly defined `SUNMatrix`.

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 8.1. It is recommended that a user-supplied SUNMATRIX implementation use the `SUNMATRIX_CUSTOM` identifier.

Table 8.2: Description of the `SUNMatrix` operations

Name	Usage and Description
SUNMatGetID	`id = SUNMatGetID(A);` Returns the type identifier for the matrix `A`. It is used to determine the matrix implementation type (e.g. dense, banded, sparse,...) from the abstract `SUNMatrix` interface. This is used to assess compatibility with SUNDIALS-provided linear solver implementations. Returned values are given in the Table 8.1.

continued on next page

Name	Usage and Description
SUNMatClone	`B = SUNMatClone(A);` Creates a new `SUNMatrix` of the same type as an existing matrix `A` and sets the *ops* field. It does not copy the matrix, but rather allocates storage for the new matrix.
SUNMatDestroy	`SUNMatDestroy(A);` Destroys the `SUNMatrix` `A` and frees memory allocated for its internal data.
SUNMatSpace	`ier = SUNMatSpace(A, &lrw, &liw);` Returns the storage requirements for the matrix `A`. `lrw` is a `long int` containing the number of realtype words and `liw` is a `long int` containing the number of integer words. The return value is an integer flag denoting success/failure of the operation. This function is advisory only, for use in determining a user's total space requirements; it could be a dummy function in a user-supplied SUNMATRIX module if that information is not of interest.
SUNMatZero	`ier = SUNMatZero(A);` Performs the operation $A_{ij} = 0$ for all entries of the matrix A. The return value is an integer flag denoting success/failure of the operation.
SUNMatCopy	`ier = SUNMatCopy(A,B);` Performs the operation $B_{ij} = A_{i,j}$ for all entries of the matrices A and B. The return value is an integer flag denoting success/failure of the operation.
SUNMatScaleAdd	`ier = SUNMatScaleAdd(c, A, B);` Performs the operation $A = cA + B$. The return value is an integer flag denoting success/failure of the operation.
SUNMatScaleAddI	`ier = SUNMatScaleAddI(c, A);` Performs the operation $A = cA + I$. The return value is an integer flag denoting success/failure of the operation.
SUNMatMatvec	`ier = SUNMatMatvec(A, x, y);` Performs the matrix-vector product operation, $y = Ax$. It should only be called with vectors `x` and `y` that are compatible with the matrix `A` – both in storage type and dimensions. The return value is an integer flag denoting success/failure of the operation.

We note that not all SUNMATRIX types are compatible with all NVECTOR types provided with SUNDIALS. This is primarily due to the need for compatibility within the `SUNMatMatvec` routine; however, compatibility between SUNMATRIX and NVECTOR implementations is more crucial when considering their interaction within SUNLINSOL objects, as will be described in more detail in Chapter 9. More specifically, in Table 8.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 8.3: SUNDIALS matrix interfaces and vector implementations that can be used for each.

Matrix Interface	Serial	Parallel (MPI)	OpenMP	pThreads	*hypre* Vec.	PETSc Vec.	CUDA	RAJA	User Suppl.
Dense	✓		✓	✓					✓

continued on next page

Matrix Interface	Serial	Parallel (MPI)	OpenMP	pThreads	*hypre* Vec.	PETSc Vec.	CUDA	RAJA	User Suppl.
Band	✓		✓	✓					✓
Sparse	✓		✓	✓					✓
User supplied	✓	✓	✓	✓	✓	✓	✓	✓	✓

8.1 The SUNMatrix_Dense implementation

The dense implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_DENSE, defines the *content* field of `SUNMatrix` to be the following structure:

```
struct _SUNMatrixContent_Dense {
  sunindextype M;
  sunindextype N;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

These entries of the *content* field contain the following information:

M - number of rows

N - number of columns

data - pointer to a contiguous block of `realtype` variables. The elements of the dense matrix are stored columnwise, i.e. the (`i`,`j`)-th element of a dense SUNMATRIX `A` (with $0 \le$ `i` $<$ `M` and $0 \le$ `j` $<$ `N`) may be accessed via `data[j*M+i]`.

ldata - length of the data array (= `M`·`N`).

cols - array of pointers. `cols[j]` points to the first element of the j-th column of the matrix in the array `data`. The (`i`,`j`)-th element of a dense SUNMATRIX `A` (with $0 \le$ `i` $<$ `M` and $0 \le$ `j` $<$ `N`) may be accessed via `cols[j][i]`.

The header file to be included when using this module is `sunmatrix/sunmatrix_dense.h`.

The following macros are provided to access the content of a SUNMATRIX_DENSE matrix. The prefix `SM_` in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix `_D` denotes that these are specific to the *dense* version.

- `SM_CONTENT_D`

  This macro gives access to the contents of the dense `SUNMatrix`.

  The assignment `A_cont` = `SM_CONTENT_D(A)` sets `A_cont` to be a pointer to the dense `SUNMatrix` content structure.

  Implementation:

  ```
  #define SM_CONTENT_D(A)     ( (SUNMatrixContent_Dense)(A->content) )
  ```

- `SM_ROWS_D`, `SM_COLUMNS_D`, and `SM_LDATA_D`

  These macros give individual access to various lengths relevant to the content of a dense `SUNMatrix`.

  These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_D(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_D(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

Implementation:

```
#define SM_ROWS_D(A)        ( SM_CONTENT_D(A)->M )
#define SM_COLUMNS_D(A)     ( SM_CONTENT_D(A)->N )
#define SM_LDATA_D(A)       ( SM_CONTENT_D(A)->ldata )
```

- SM_DATA_D and SM_COLS_D

  These macros give access to the data and cols pointers for the matrix entries.

  The assignment A_data = SM_DATA_D(A) sets A_data to be a pointer to the first component of the data array for the dense SUNMatrix A. The assignment SM_DATA_D(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_cols = SM_COLS_D(A) sets A_cols to be a pointer to the array of column pointers for the dense SUNMatrix A. The assignment SM_COLS_D(A) = A_cols sets the column pointer array of A to be A_cols by storing the pointer A_cols.

  Implementation:

  ```
  #define SM_DATA_D(A)        ( SM_CONTENT_D(A)->data )
  #define SM_COLS_D(A)        ( SM_CONTENT_D(A)->cols )
  ```

- SM_COLUMN_D and SM_ELEMENT_D

  These macros give access to the individual columns and entries of the data array of a dense SUNMatrix.

  The assignment col_j = SM_COLUMN_D(A,j) sets col_j to be a pointer to the first entry of the j-th column of the M × N dense matrix A (with $0 \le j < N$). The type of the expression SM_COLUMN_D(A,j) is realtype *. The pointer returned by the call SM_COLUMN_D(A,j) can be treated as an array which is indexed from 0 to $M - 1$.

  The assignments SM_ELEMENT_D(A,i,j) = a_ij and a_ij = SM_ELEMENT_D(A,i,j) reference the (i,j)-th element of the M × N dense matrix A (with $0 \le i < M$ and $0 \le j < N$).

  Implementation:

  ```
  #define SM_COLUMN_D(A,j)    ( (SM_CONTENT_D(A)->cols)[j] )
  #define SM_ELEMENT_D(A,i,j) ( (SM_CONTENT_D(A)->cols)[j][i] )
  ```

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Table 8.2. Their names are obtained from those in Table 8.2 by appending the suffix _Dense (e.g. SUNMatCopy_Dense). The module SUNMATRIX_DENSE provides the following additional user-callable routines:

- SUNDenseMatrix

  This constructor function creates and allocates memory for a dense SUNMatrix. Its arguments are the number of rows, M, and columns, N, for the dense matrix.

  ```
  SUNMatrix SUNDenseMatrix(sunindextype M, sunindextype N);
  ```

- SUNDenseMatrix_Print

  This function prints the content of a dense SUNMatrix to the output stream specified by outfile. Note: stdout or stderr may be used as arguments for outfile to print directly to standard output or standard error, respectively.

  ```
  void SUNDenseMatrix_Print(SUNMatrix A, FILE* outfile);
  ```

- SUNDenseMatrix_Rows

  This function returns the number of rows in the dense SUNMatrix.

  ```
  sunindextype SUNDenseMatrix_Rows(SUNMatrix A);
  ```

- `SUNDenseMatrix_Columns`

  This function returns the number of columns in the dense `SUNMatrix`.

  ```
  sunindextype SUNDenseMatrix_Columns(SUNMatrix A);
  ```

- `SUNDenseMatrix_LData`

  This function returns the length of the data array for the dense `SUNMatrix`.

  ```
  sunindextype SUNDenseMatrix_LData(SUNMatrix A);
  ```

- `SUNDenseMatrix_Data`

  This function returns a pointer to the data array for the dense `SUNMatrix`.

  ```
  realtype* SUNDenseMatrix_Data(SUNMatrix A);
  ```

- `SUNDenseMatrix_Cols`

  This function returns a pointer to the cols array for the dense `SUNMatrix`.

  ```
  realtype** SUNDenseMatrix_Cols(SUNMatrix A);
  ```

- `SUNDenseMatrix_Column`

  This function returns a pointer to the first entry of the jth column of the dense `SUNMatrix`. The resulting pointer should be indexed over the range 0 to `M` $-$ 1.

  ```
  realtype* SUNDenseMatrix_Column(SUNMatrix A, sunindextype j);
  ```

Notes

- When looping over the components of a dense `SUNMatrix A`, the most efficient approaches are to:

  – First obtain the component array via `A_data = SM_DATA_D(A)` or `A_data = SUNDenseMatrix_Data(A)` and then access `A_data[i]` within the loop.

  – First obtain the array of column pointers via `A_cols = SM_COLS_D(A)` or `A_cols = SUNDenseMatrix_Cols(A)`, and then access `A_cols[j][i]` within the loop.

  – Within a loop over the columns, access the column pointer via `A_colj = SUNDenseMatrix_Column(A,j)` and then to access the entries within that column using `A_colj[i]` within the loop.

  All three of these are more efficient than using `SM_ELEMENT_D(A,i,j)` within a double loop.

- Within the `SUNMatMatvec_Dense` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

For solvers that include a Fortran interface module, the SUNMATRIX_DENSE module also includes the Fortran-callable function `FSUNDenseMatInit(code, M, N, ier)` to initialize this SUNMATRIX_DENSE module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `M` and `N` are the corresponding dense matrix construction arguments (declared to match C type `long int`); and `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNDenseMassMatInit(M, N, ier)` initializes this SUNMATRIX_DENSE module for storing the mass matrix.

8.2 The SUNMatrix_Band implementation

The banded implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_BAND, defines the *content* field of `SUNMatrix` to be the following structure:

```
struct _SUNMatrixContent_Band {
  sunindextype M;
  sunindextype N;
  sunindextype mu;
  sunindextype ml;
  sunindextype s_mu;
  sunindextype ldim;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

A diagram of the underlying data representation in a banded matrix is shown in Figure 8.1. A more complete description of the parts of this *content* field is given below:

M - number of rows

N - number of columns (`N` = `M`)

mu - upper half-bandwidth, 0 ≤ `mu` < `N`

ml - lower half-bandwidth, 0 ≤ `ml` < `N`

s_mu - storage upper bandwidth, `mu` ≤ `s_mu` < `N`. The LU decomposition routines in the associated SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(`N`-1,`mu`+`ml`) because of partial pivoting. The `s_mu` field holds the upper half-bandwidth allocated for A.

ldim - leading dimension (`ldim` ≥ `s_mu`)

data - pointer to a contiguous block of `realtype` variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. `data` is a pointer to `ldata` contiguous locations which hold the elements within the band of A.

ldata - length of the data array (= `ldim`·(`s_mu`+`ml`+1))

cols - array of pointers. `cols[j]` is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from `s_mu`−`mu` (to access the uppermost element within the band in the j-th column) to `s_mu`+`ml` (to access the lowest element within the band in the j-th column). Indices from 0 to `s_mu`−`mu`−1 give access to extra storage elements required by the LU decomposition function. Finally, `cols[j][i-j+s_mu]` is the (i, j)-th element with j−`mu` ≤ i ≤ j+`ml`.

The header file to be included when using this module is `sunmatrix/sunmatrix_band.h`.

The following macros are provided to access the content of a SUNMATRIX_BAND matrix. The prefix `SM_` in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix `_B` denotes that these are specific to the *banded* version.

- `SM_CONTENT_B`

  This routine gives access to the contents of the banded `SUNMatrix`.

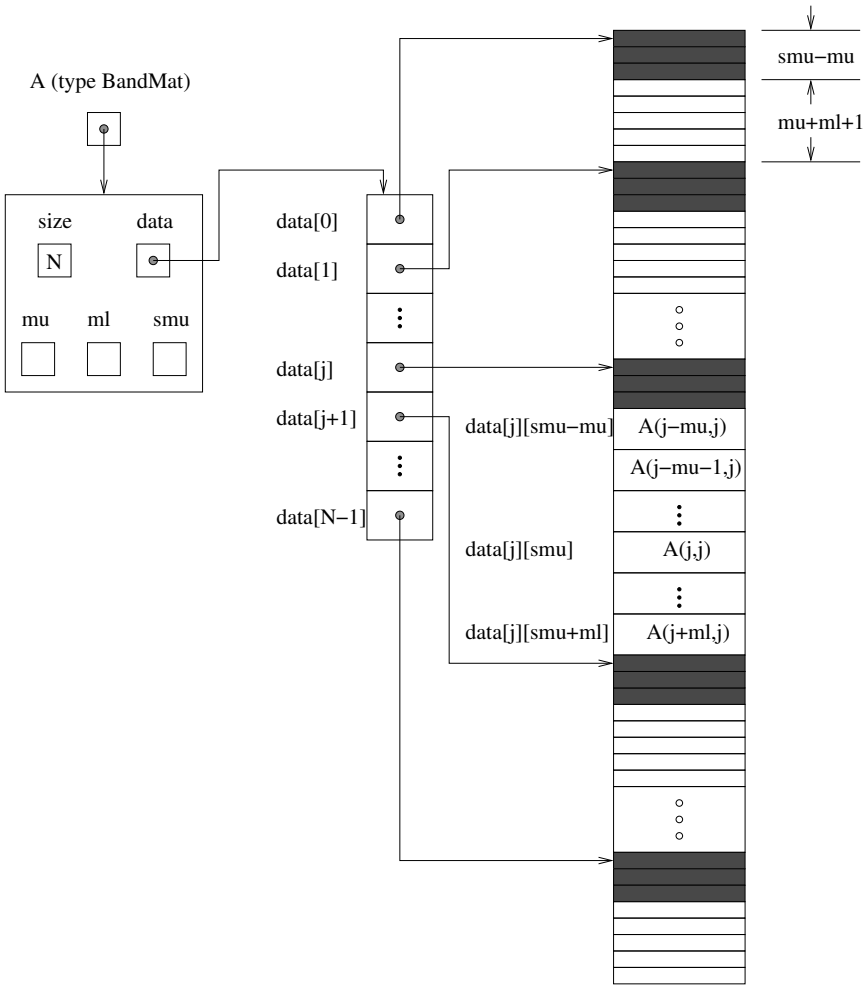

Figure 8.1: Diagram of the storage for the SUNMATRIX_BAND module. Here `A` is an $\texttt{N} \times \texttt{N}$ band matrix with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to $\texttt{N} - 1$ and the (i, j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the associated SUNLINSOL_BAND linear solver.

The assignment A_cont = SM_CONTENT_B(A) sets A_cont to be a pointer to the banded SUNMatrix content structure.

Implementation:

```
#define SM_CONTENT_B(A)     ( (SUNMatrixContent_Band)(A->content) )
```

- SM_ROWS_B, SM_COLUMNS_B, SM_UBAND_B, SM_LBAND_B, SM_SUBAND_B, SM_LDIM_B, and SM_LDATA_B

  These macros give individual access to various lengths relevant to the content of a banded SUNMatrix.

  These may be used either to retrieve or to set these values. For example, the assignment A_rows = SM_ROWS_B(A) sets A_rows to be the number of rows in the matrix A. Similarly, the assignment SM_COLUMNS_B(A) = A_cols sets the number of columns in A to equal A_cols.

  Implementation:

```
#define SM_ROWS_B(A)        ( SM_CONTENT_B(A)->M )
#define SM_COLUMNS_B(A)     ( SM_CONTENT_B(A)->N )
#define SM_UBAND_B(A)       ( SM_CONTENT_B(A)->mu )
#define SM_LBAND_B(A)       ( SM_CONTENT_B(A)->ml )
#define SM_SUBAND_B(A)      ( SM_CONTENT_B(A)->s_mu )
#define SM_LDIM_B(A)        ( SM_CONTENT_B(A)->ldim )
#define SM_LDATA_B(A)       ( SM_CONTENT_B(A)->ldata )
```

- SM_DATA_B and SM_COLS_B

  These macros give access to the data and cols pointers for the matrix entries.

  The assignment A_data = SM_DATA_B(A) sets A_data to be a pointer to the first component of the data array for the banded SUNMatrix A. The assignment SM_DATA_B(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_cols = SM_COLS_B(A) sets A_cols to be a pointer to the array of column pointers for the banded SUNMatrix A. The assignment SM_COLS_B(A) = A_cols sets the column pointer array of A to be A_cols by storing the pointer A_cols.

  Implementation:

```
#define SM_DATA_B(A)        ( SM_CONTENT_B(A)->data )
#define SM_COLS_B(A)        ( SM_CONTENT_B(A)->cols )
```

- SM_COLUMN_B, SM_COLUMN_ELEMENT_B, and SM_ELEMENT_B

  These macros give access to the individual columns and entries of the data array of a banded SUNMatrix.

  The assignments SM_ELEMENT_B(A,i,j) = a_ij and a_ij = SM_ELEMENT_B(A,i,j) reference the (i,j)-th element of the N × N band matrix A, where $0 \le$ i, j $\le$ N − 1. The location (i,j) should further satisfy j−mu $\le$ i $\le$ j+ml.

  The assignment col_j = SM_COLUMN_B(A,j) sets col_j to be a pointer to the diagonal element of the j-th column of the N × N band matrix A, $0 \le$ j $\le$ N − 1. The type of the expression SM_COLUMN_B(A,j) is realtype *. The pointer returned by the call SM_COLUMN_B(A,j) can be treated as an array which is indexed from −mu to ml.

  The assignments SM_COLUMN_ELEMENT_B(col_j,i,j) = a_ij and a_ij = SM_COLUMN_ELEMENT_B(col_j,i,j) reference the (i,j)-th entry of the band matrix A when used in conjunction with SM_COLUMN_B to reference the j-th column through col_j. The index (i,j) should satisfy j−mu $\le$ i $\le$ j+ml.

  Implementation:

```
#define SM_COLUMN_B(A,j)    ( ((SM_CONTENT_B(A)->cols)[j])+SM_SUBAND_B(A) )
#define SM_COLUMN_ELEMENT_B(col_j,i,j) (col_j[(i)-(j)])
#define SM_ELEMENT_B(A,i,j)
              ( (SM_CONTENT_B(A)->cols)[j][(i)-(j)+SM_SUBAND_B(A)] )
```

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Table 8.2. Their names are obtained from those in Table 8.2 by appending the suffix `_Band` (e.g. `SUNMatCopy_Band`). The module SUNMATRIX_BAND provides the following additional user-callable routines:

- `SUNBandMatrix`

  This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, the upper and lower half-bandwidths of the matrix, `mu` and `ml`, and the stored upper bandwidth, `smu`. When creating a band `SUNMatrix`, if the matrix will be used by the SUNLINSOL_BAND module then `smu` should be at least min(`N`-1,`mu`+`ml`); otherwise `smu` should be at least `mu`.

  ```
  SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu,
                          sunindextype ml, sunindextype smu);
  ```

- `SUNBandMatrix_Print`

  This function prints the content of a banded `SUNMatrix` to the output stream specified by `outfile`. Note: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

  ```
  void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile);
  ```

- `SUNBandMatrix_Rows`

  This function returns the number of rows in the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_Rows(SUNMatrix A);
  ```

- `SUNBandMatrix_Columns`

  This function returns the number of columns in the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_Columns(SUNMatrix A);
  ```

- `SUNBandMatrix_LowerBandwidth`

  This function returns the lower half-bandwidth of the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A);
  ```

- `SUNBandMatrix_UpperBandwidth`

  This function returns the upper half-bandwidth of the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A);
  ```

- `SUNBandMatrix_StoredUpperBandwidth`

  This function returns the stored upper half-bandwidth of the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A);
  ```

- `SUNBandMatrix_LDim`

  This function returns the length of the leading dimension of the banded `SUNMatrix`.

  ```
  sunindextype SUNBandMatrix_LDim(SUNMatrix A);
  ```

- SUNBandMatrix_Data

  This function returns a pointer to the data array for the banded SUNMatrix.

  ```
  realtype* SUNBandMatrix_Data(SUNMatrix A);
  ```

- SUNBandMatrix_Cols

  This function returns a pointer to the cols array for the banded SUNMatrix.

  ```
  realtype** SUNBandMatrix_Cols(SUNMatrix A);
  ```

- SUNBandMatrix_Column

  This function returns a pointer to the diagonal entry of the j-th column of the banded SUNMatrix. The resulting pointer should be indexed over the range $-$mu to ml.

  ```
  realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j);
  ```

Notes

- When looping over the components of a banded SUNMatrix A, the most efficient approaches are to:
  - First obtain the component array via A_data = SM_DATA_B(A) or A_data = SUNBandMatrix_Data(A) and then access A_data[i] within the loop.
  - First obtain the array of column pointers via A_cols = SM_COLS_B(A) or A_cols = SUNBandMatrix_Cols(A), and then access A_cols[j][i] within the loop.
  - Within a loop over the columns, access the column pointer via A_colj = SUNBandMatrix_Column(A,j) and then to access the entries within that column using SM_COLUMN_ELEMENT_B(A_colj,i,j).

  All three of these are more efficient than using SM_ELEMENT_B(A,i,j) within a double loop.

- Within the SUNMatMatvec_Band routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

For solvers that include a Fortran interface module, the SUNMATRIX_BAND module also includes the Fortran-callable function FSUNBandMatInit(code, N, mu, ml, smu, ier) to initialize this SUNMATRIX_BAND module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); N, mu, ml and smu are the corresponding band matrix construction arguments (declared to match C type long int); and ier is an error return flag equal to 0 for success and -1 for failure. Both code and ier are declared to match C type int. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function FSUNBandMassMatInit(N, mu, ml, smu, ier) initializes this SUNMATRIX_BAND module for storing the mass matrix.

8.3 The SUNMatrix_Sparse implementation

The sparse implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_SPARSE, is designed to work with either *compressed-sparse-column* (CSC) or *compressed-sparse-row* (CSR) sparse matrix formats. To this end, it defines the *content* field of SUNMatrix to be the following structure:

```
struct _SUNMatrixContent_Sparse {
  sunindextype M;
  sunindextype N;
  sunindextype NNZ;
```

```
  sunindextype NP;
  realtype *data;
  int sparsetype;
  sunindextype *indexvals;
  sunindextype *indexptrs;
  /* CSC indices */
  sunindextype **rowvals;
  sunindextype **colptrs;
  /* CSR indices */
  sunindextype **colvals;
  sunindextype **rowptrs;
};
```

A diagram of the underlying data representation for a CSC matrix is shown in Figure 8.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

M - number of rows

N - number of columns

NNZ - maximum number of nonzero entries in the matrix (allocated length of `data` and `indexvals` arrays)

NP - number of index pointers (e.g. number of column pointers for CSC matrix). For CSC matrices `NP` = `N`, and for CSR matrices `NP` = `M`. This value is set automatically based the input for `sparsetype`.

data - pointer to a contiguous block of `realtype` variables (of length `NNZ`), containing the values of the nonzero entries in the matrix

sparsetype - type of the sparse matrix (`CSC_MAT` or `CSR_MAT`)

indexvals - pointer to a contiguous block of `int` variables (of length `NNZ`), containing the row indices (if CSC) or column indices (if CSR) of each nonzero matrix entry held in `data`

indexptrs - pointer to a contiguous block of `int` variables (of length `NP+1`). For CSC matrices each entry provides the index of the first column entry into the `data` and `indexvals` arrays, e.g. if `indexptr[3]=7`, then the first nonzero entry in the fourth column of the matrix is located in `data[7]`, and is located in row `indexvals[7]` of the matrix. The last entry contains the total number of nonzero values in the matrix and hence points one past the end of the active data in the `data` and `indexvals` arrays. For CSR matrices, each entry provides the index of the first row entry into the `data` and `indexvals` arrays.

The following pointers are added to the `SlsMat` type for user convenience, to provide a more intuitive interface to the CSC and CSR sparse matrix data structures. They are set automatically when creating a sparse SUNMATRIX, based on the sparse matrix storage type.

rowvals - pointer to `indexvals` when `sparsetype` is `CSC_MAT`, otherwise set to `NULL`.

colptrs - pointer to `indexptrs` when `sparsetype` is `CSC_MAT`, otherwise set to `NULL`.

colvals - pointer to `indexvals` when `sparsetype` is `CSR_MAT`, otherwise set to `NULL`.

rowptrs - pointer to `indexptrs` when `sparsetype` is `CSR_MAT`, otherwise set to `NULL`.

For example, the 5×4 CSC matrix

$$\begin{bmatrix} 0 & 3 & 1 & 0 \\ 3 & 0 & 0 & 2 \\ 0 & 7 & 0 & 0 \\ 1 & 0 & 0 & 9 \\ 0 & 0 & 0 & 5 \end{bmatrix}$$

could be stored in this structure as either

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4};
indexptrs = {0, 2, 4, 5, 8};
```

or

```
M = 5;
N = 4;
NNZ = 10;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0, *, *};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4, *, *};
indexptrs = {0, 2, 4, 5, 8};
```

where the first has no unused space, and the second has additional storage (the entries marked with * may contain any values). Note in both cases that the final value in `indexptrs` is 8, indicating the total number of nonzero entries in the matrix.

Similarly, in CSR format, the same matrix could be stored as

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 2.0, 7.0, 1.0, 9.0, 5.0};
sparsetype = CSR_MAT;
indexvals = {1, 2, 0, 3, 1, 0, 3, 3};
indexptrs = {0, 2, 4, 5, 7, 8};
```

The header file to be included when using this module is `sunmatrix/sunmatrix_sparse.h`.

The following macros are provided to access the content of a SUNMATRIX_SPARSE matrix. The prefix `SM_` in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix `_S` denotes that these are specific to the *sparse* version.

- `SM_CONTENT_S`

  This routine gives access to the contents of the sparse `SUNMatrix`.

  The assignment `A_cont = SM_CONTENT_S(A)` sets `A_cont` to be a pointer to the sparse `SUNMatrix` content structure.

  Implementation:

  ```
  #define SM_CONTENT_S(A)     ( (SUNMatrixContent_Sparse)(A->content) )
  ```

- `SM_ROWS_S`, `SM_COLUMNS_S`, `SM_NNZ_S`, `SM_NP_S`, and `SM_SPARSETYPE_S`

  These macros give individual access to various lengths relevant to the content of a sparse `SUNMatrix`.

  These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_S(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_S(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

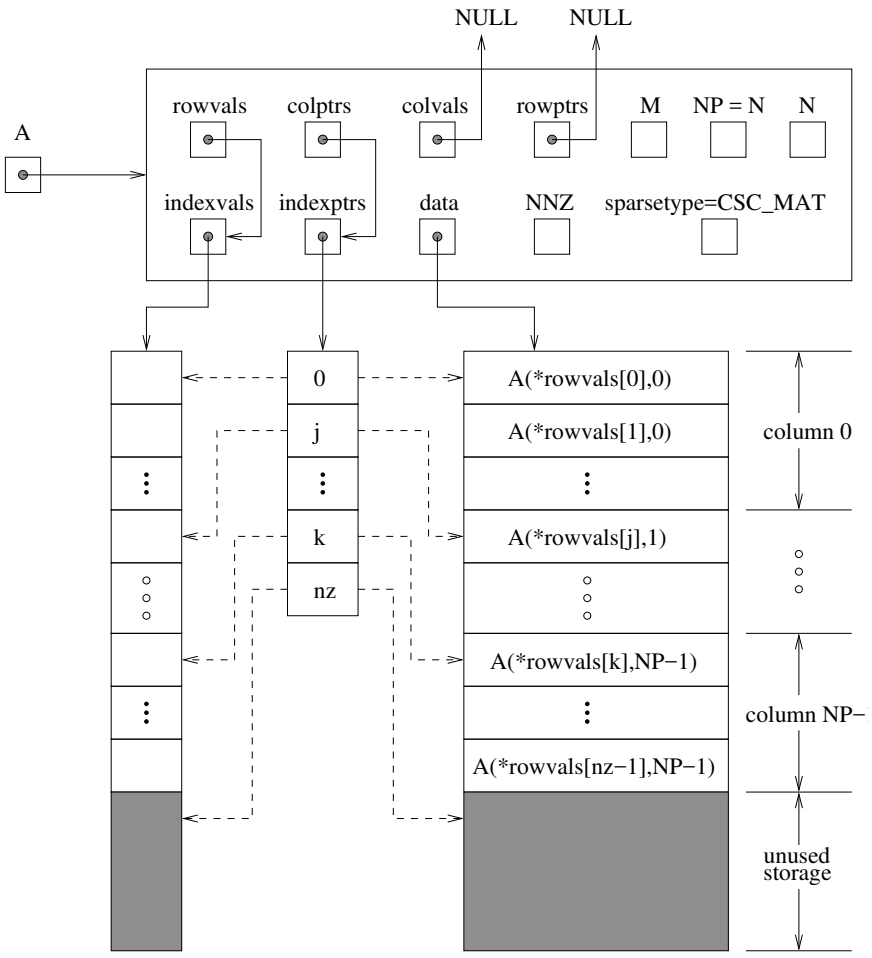

Figure 8.2: Diagram of the storage for a compressed-sparse-column matrix. Here `A` is an $\texttt{M} \times \texttt{N}$ sparse matrix with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to $\texttt{M} - 1$, corresponding to the row index (zero-based) of each nonzero value. The entries in `data` contain the values of the nonzero entries, with the row i, column j entry of `A` (again, zero-based) denoted as `A(i,j)`. The `indexptrs` array contains $\texttt{N}+1$ entries; the first `N` denote the starting index of each column within the `indexvals` and `data` arrays, while the final entry points one past the final nonzero entry. Here, although `NNZ` values are allocated, only `nz` are actually filled in; the greyed-out portions of `data` and `indexvals` indicate extra allocated space.

Implementation:

```
#define SM_ROWS_S(A)        ( SM_CONTENT_S(A)->M )
#define SM_COLUMNS_S(A)     ( SM_CONTENT_S(A)->N )
#define SM_NNZ_S(A)         ( SM_CONTENT_S(A)->NNZ )
#define SM_NP_S(A)          ( SM_CONTENT_S(A)->NP )
#define SM_SPARSETYPE_S(A)  ( SM_CONTENT_S(A)->sparsetype )
```

- SM_DATA_S, SM_INDEXVALS_S, and SM_INDEXPTRS_S

  These macros give access to the data and index arrays for the matrix entries.

  The assignment A_data = SM_DATA_S(A) sets A_data to be a pointer to the first component of the data array for the sparse SUNMatrix A. The assignment SM_DATA_S(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_indexvals = SM_INDEXVALS_S(A) sets A_indexvals to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix A. The assignment A_indexptrs = SM_INDEXPTRS_S(A) sets A_indexptrs to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).

  Implementation:

```
#define SM_DATA_S(A)        ( SM_CONTENT_S(A)->data )
#define SM_INDEXVALS_S(A)   ( SM_CONTENT_S(A)->indexvals )
#define SM_INDEXPTRS_S(A)   ( SM_CONTENT_S(A)->indexptrs )
```

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Table 8.2. Their names are obtained from those in Table 8.2 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). The module SUNMATRIX_SPARSE provides the following additional user-callable routines:

- SUNSparseMatrix

  This function creates and allocates memory for a sparse SUNMatrix. Its arguments are the number of rows and columns of the matrix, M and N, the maximum number of nonzeros to be stored in the matrix, NNZ, and a flag sparsetype indicating whether to use CSR or CSC format (valid arguments are CSR_MAT or CSC_MAT).

```
SUNMatrix SUNSparseMatrix(sunindextype M, sunindextype N,
                          sunindextype NNZ, int sparsetype);
```

- SUNSparseFromDenseMatrix

  This function creates a new sparse matrix from an existing dense matrix by copying all values with magnitude larger than droptol into the sparse matrix structure.

  Requirements:

  – A must have type SUNMATRIX_DENSE;

  – droptol must be non-negative;

  – sparsetype must be either CSC_MAT or CSR_MAT.

  The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

```
SUNMatrix SUNSparseFromDenseMatrix(SUNMatrix A, realtype droptol,
                                   int sparsetype);
```

- SUNSparseFromBandMatrix

  This function creates a new sparse matrix from an existing band matrix by copying all values with magnitude larger than `droptol` into the sparse matrix structure.

  Requirements:

  - `A` must have type `SUNMATRIX_BAND`;
  - `droptol` must be non-negative;
  - `sparsetype` must be either `CSC_MAT` or `CSR_MAT`.

  The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

  ```
  SUNMatrix SUNSparseFromBandMatrix(SUNMatrix A, realtype droptol,
                                    int sparsetype);
  ```

- SUNSparseMatrix_Realloc

  This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has no wasted space (i.e. the space allocated for nonzero entries equals the actual number of nonzeros, `indexptrs[NP]`). Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse).

  ```
  int SUNSparseMatrix_Realloc(SUNMatrix A);
  ```

- SUNSparseMatrix_Print

  This function prints the content of a sparse `SUNMatrix` to the output stream specified by `outfile`. Note: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

  ```
  void SUNSparseMatrix_Print(SUNMatrix A, FILE* outfile);
  ```

- SUNSparseMatrix_Rows

  This function returns the number of rows in the sparse `SUNMatrix`.

  ```
  sunindextype SUNSparseMatrix_Rows(SUNMatrix A);
  ```

- SUNSparseMatrix_Columns

  This function returns the number of columns in the sparse `SUNMatrix`.

  ```
  sunindextype SUNSparseMatrix_Columns(SUNMatrix A);
  ```

- SUNSparseMatrix_NNZ

  This function returns the number of entries allocated for nonzero storage for the sparse matrix `SUNMatrix`.

  ```
  sunindextype SUNSparseMatrix_NNZ(SUNMatrix A);
  ```

- SUNSparseMatrix_NP

  This function returns the number of columns/rows for the sparse `SUNMatrix`, depending on whether the matrix uses CSC/CSR format, respectively. The `indexptrs` array has `NP+1` entries.

  ```
  sunindextype SUNSparseMatrix_NP(SUNMatrix A);
  ```

- SUNSparseMatrix_SparseType

  This function returns the storage type (CSR_MAT or CSC_MAT) for the sparse SUNMatrix.

  ```
  int SUNSparseMatrix_SparseType(SUNMatrix A);
  ```

- SUNSparseMatrix_Data

  This function returns a pointer to the data array for the sparse SUNMatrix.

  ```
  realtype* SUNSparseMatrix_Data(SUNMatrix A);
  ```

- SUNSparseMatrix_IndexValues

  This function returns a pointer to index value array for the sparse SUNMatrix: for CSR format this is the column index for each nonzero entry, for CSC format this is the row index for each nonzero entry.

  ```
  sunindextype* SUNSparseMatrix_IndexValues(SUNMatrix A);
  ```

- SUNSparseMatrix_IndexPointers

  This function returns a pointer to the index pointer array for the sparse SUNMatrix: for CSR format this is the location of the first entry of each row in the data and indexvalues arrays, for CSC format this is the location of the first entry of each column.

  ```
  sunindextype* SUNSparseMatrix_IndexPointers(SUNMatrix A);
  ```


Within the SUNMatMatvec_Sparse routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

For solvers that include a Fortran interface module, the SUNMATRIX_SPARSE module also includes the Fortran-callable function `FSUNSparseMatInit(code, M, N, NNZ, sparsetype, ier)` to initialize this SUNMATRIX_SPARSE module for a given SUNDIALS solver. Here `code` is an integer input for the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `M`, `N` and `NNZ` are the corresponding sparse matrix construction arguments (declared to match C type `long int`); `sparsetype` is an integer flag indicating the sparse storage type (0 for CSC, 1 for CSR); and `ier` is an error return flag equal to 0 for success and -1 for failure. Each of `code`, `sparsetype` and `ier` are declared so as to match C type `int`. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNSparseMassMatInit(M, N, NNZ, sparsetype, ier)` initializes this SUNMATRIX_SPARSE module for storing the mass matrix.

8.4 SUNMatrix Examples

There are SUNMatrix examples that may be installed for each implementation: dense, banded, and sparse. Each implementation makes use of the functions in `test_sunmatrix.c`. These example functions show simple usage of the SUNMatrix family of functions. The inputs to the examples depend on the matrix type, and are output to `stdout` if the example is run without the appropriate number of command-line arguments.
The following is a list of the example functions in `test_sunmatrix.c`:

- `Test_SUNMatGetID`: Verifies the returned matrix ID against the value that should be returned.
- `Test_SUNMatClone`: Creates clone of an existing matrix, copies the data, and checks that their values match.
- `Test_SUNMatZero`: Zeros out an existing matrix and checks that each entry equals 0.0.
- `Test_SUNMatCopy`: Clones an input matrix, copies its data to a clone, and verifies that all values match.

- `Test_SUNMatScaleAdd`: Given an input matrix A and an input identity matrix I, this test clones and copies A to a new matrix B, computes $B = -B + B$, and verifies that the resulting matrix entries equal 0.0. Additionally, if the matrix is square, this test clones and copies A to a new matrix D, clones and copies I to a new matrix C, computes $D = D + I$ and $C = C + A$ using `SUNMatScaleAdd`, and then verifies that $C == D$.

- `Test_SUNMatScaleAddI`: Given an input matrix A and an input identity matrix I, this clones and copies I to a new matrix B, computes $B = -B + I$ using `SUNMatScaleAddI`, and verifies that the resulting matrix entries equal 0.0.

- `Test_SUNMatMatvec` Given an input matrix A and input vectors x and y such that $y = Ax$, this test has different behavior depending on whether A is square. If it is square, it clones and copies A to a new matrix B, computes $B = 3B + I$ using `SUNMatScaleAddI`, clones y to new vectors w and z, computes $z = Bx$ using `SUNMatMatvec`, computes $w = 3y + x$ using `N_VLinearSum`, and verifies that $w == z$. If A is not square, it just clones y to a new vector z, computes $z = Ax$ using `SUNMatMatvec`, and verifies that $y == z$.

- `Test_SUNMatSpace` verifies that `SUNMatSpace` can be called, and outputs the results to `stdout`.

8.5 SUNMatrix functions used by IDAS

In Table 8.4 below, we list the matrix functions in the SUNMATRIX module used within the IDAS package. The table also shows, for each function, which of the code modules uses the function. Neither the main IDAS integrator or the IDASPILS interface call SUNMATRIX functions directly, so the table columns are specific to the IDADLS direct solver interface and the IDABBDPRE preconditioner module.

At this point, we should emphasize that the IDAS user does not need to know anything about the usage of matrix functions by the IDAS code modules in order to use IDAS. The information is presented as an implementation detail for the interested reader.

Table 8.4: List of matrix functions usage by IDAS code modules

	IDADLS	IDABBDPRE
SUNMatGetID	✓	
SUNMatDestroy		✓
SUNMatZero	✓	✓
SUNMatSpace		†

The matrix functions listed in Table 8.2 with a † symbol are optionally used, in that these are only called if they are implemented in the SUNMATRIX module that is being used (i.e. their function pointers are non-`NULL`). The matrix functions listed in Table 8.2 that are *not* used by IDAS are: `SUNMatCopy`, `SUNMatClone`, `SUNMatScaleAdd`, `SUNMatScaleAddI` and `SUNMatMatvec`. Therefore a user-supplied SUNMATRIX module for IDAS could omit these functions.

Chapter 9

Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS solvers operate using generic linear solver modules (of type `SUNLinearSolver`), through a set of operations defined by the particular SUNLINSOL implementation. These work in coordination with the SUNDIALS generic NVECTOR and SUNMATRIX modules to provide a set of compatible data structures and solvers for the solution of linear systems using direct or iterative methods. Moreover, users can provide their own specific SUNLINSOL implementation to each SUNDIALS solver, particularly in cases where they provide their own NVECTOR and/or SUNMATRIX modules, and the customized linear solver leverages these additional data structures to create highly efficient and/or scalable solvers for their particular problem. Additionally, SUNDIALS provides native implementations SUNLINSOL modules, as well as SUNLINSOL modules that interface between SUNDIALS and external linear solver libraries.

The various SUNDIALS solvers have been designed to specifically leverage the use of either *direct linear solvers* or *scaled, preconditioned, iterative linear solvers*, through their "Dls" and "Spils" interfaces, respectively. Additionally, SUNDIALS solvers can make use of user-supplied custom linear solvers, whether these are problem-specific or come from external solver libraries.

For iterative (and possibly custom) linear solvers, the SUNDIALS solvers leverage scaling and preconditioning, as applicable, to balance error between solution components and to accelerate convergence of the linear solver. To this end, instead of solving the linear system $Ax = b$ directly, we apply the underlying iterative algorithm to the transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.1}$$

where

$$\begin{aligned} \tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\ \tilde{b} &= S_1 P_1^{-1} b, \\ \tilde{x} &= S_2 P_2 x, \end{aligned} \tag{9.2}$$

and where

- P_1 is the left preconditioner,
- P_2 is the right preconditioner,
- S_1 is a diagonal matrix of scale factors for $P_1^{-1}b$,
- S_2 is a diagonal matrix of scale factors for $P_2 x$.

The SUNDIALS solvers request that iterative linear solvers stop based on the 2-norm of the scaled preconditioned residual meeting a prescribed tolerance

$$\left\| \tilde{b} - \tilde{A}\tilde{x} \right\|_2 < \text{tol}.$$

We note that not all of the iterative linear solvers implemented in SUNDIALS support the full range of the above options. Similarly, some of the SUNDIALS integrators only utilize a subset of these options. Exceptions to the operators shown above are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS solver "Spils" interface.

The generic `SUNLinearSolver` type has been modeled after the object-oriented style of the generic `N_Vector` type. Specifically, a generic `SUNLinearSolver` is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the linear solver, and an *ops* field pointing to a structure with generic linear solver operations. The type `SUNLinearSolver` is defined as

```
typedef struct _generic_SUNLinearSolver *SUNLinearSolver;

struct _generic_SUNLinearSolver {
  void *content;
  struct _generic_SUNLinearSolver_Ops *ops;
};
```

The `_generic_SUNLinearSolver_Ops` structure is essentially a list of pointers to the various actual linear solver operations, and is defined as

```
struct _generic_SUNLinearSolver_Ops {
  SUNLinearSolver_Type (*gettype)(SUNLinearSolver);
  int                  (*setatimes)(SUNLinearSolver, void*, ATimesFn);
  int                  (*setpreconditioner)(SUNLinearSolver, void*,
                                            PSetupFn, PSolveFn);
  int                  (*setscalingvectors)(SUNLinearSolver,
                                            N_Vector, N_Vector);
  int                  (*initialize)(SUNLinearSolver);
  int                  (*setup)(SUNLinearSolver, SUNMatrix);
  int                  (*solve)(SUNLinearSolver, SUNMatrix, N_Vector,
                                N_Vector, realtype);
  int                  (*numiters)(SUNLinearSolver);
  realtype             (*resnorm)(SUNLinearSolver);
  long int             (*lastflag)(SUNLinearSolver);
  int                  (*space)(SUNLinearSolver, long int*, long int*);
  N_Vector             (*resid)(SUNLinearSolver);
  int                  (*free)(SUNLinearSolver);
};
```

The generic SUNLINSOL module defines and implements the linear solver operations acting on `SUNLinearSolver` objects. These routines are in fact only wrappers for the linear solver operations defined by a particular SUNLINSOL implementation, which are accessed through the *ops* field of the `SUNLinearSolver` structure. To illustrate this point we show below the implementation of a typical linear solver operation from the generic SUNLINSOL module, namely `SUNLinSolInitialize`, which initializes a SUNLINSOL object for use after it has been created and configured, and returns a flag denoting a successful/failed operation:

```
int SUNLinSolInitialize(SUNLinearSolver S)
{
  return ((int) S->ops->initialize(S));
}
```

Table 9.2 contains a complete list of all linear solver operations defined by the generic SUNLINSOL module. In order to support both direct and iterative linear solver types, the generic SUNLINSOL module defines linear solver routines (or arguments) that may be specific to individual use cases. As such, for each routine we specify its intended use. If a custom SUNLINSOL module is provided, the function pointers for non-required routines may be set to `NULL` to indicate that they are not provided.

A particular implementation of the SUNLINSOL module must:

Table 9.1: Identifiers associated with linear solver kernels supplied with SUNDIALS.

Linear Solver ID	Solver type	ID Value
SUNLINEARSOLVER_DIRECT	Direct solvers	0
SUNLINEARSOLVER_ITERATIVE	Iterative solvers	1
SUNLINEARSOLVER_CUSTOM	Custom solvers	2

- Specify the *content* field of the `SUNLinearSolver` object.
- Define and implement a minimal subset of the linear solver operations. See the documentation for each SUNDIALS linear solver interface to determine which SUNLINSOL operations they require.

  Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNLINSOL module (each with different `SUNLinearSolver` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free a `SUNLinearSolver` with the new *content* field and with *ops* pointing to the new linear solver operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined `SUNLinearSolver` (e.g., routines to set various configuration options for tuning the linear solver to a particular problem).
- Optionally, provide functions as needed for that particular implementation to access different parts in the *content* field of the newly defined `SUNLinearSolver` object (e.g., routines to return various statistics from the solver).

Each SUNLINSOL implementation included in SUNDIALS has a "type" identifier specified in enumeration and shown in Table 9.1. It is recommended that a user-supplied SUNLINSOL implementation set this identifier based on the SUNDIALS solver interface they intend to use: "Dls" interfaces require the `SUNLINEARSOLVER_DIRECT` SUNLINSOL objects and "Spils" interfaces require the `SUNLINEARSOLVER_ITERATIVE` objects.

Table 9.2: Description of the `SUNLinearSolver` operations

Name	Usage and Description
`SUNLinSolGetType`	`type = SUNLinSolGetType(LS);` Returns the type identifier for the linear solver `LS`. It is used to determine the solver type (direct, iterative, or custom) from the abstract `SUNLinearSolver` interface. This is used to assess compatibility with SUNDIALS-provided linear solver interfaces. Returned values are given in the Table 9.1.

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Name	Usage and Description
SUNLinSolInitialize	`ier = SUNLinSolInitialize(LS);` Performs linear solver initialization (assumes that all solver-specific options have been set). This should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.4.
SUNLinSolSetup	`ier = SUNLinSolSetup(LS, A);` Performs any linear solver setup needed, based on an updated system SUNMATRIX `A`. This may be called frequently (e.g. with a full Newton method) or infrequently (for a modified Newton method), based on the type of integrator and/or nonlinear solver requesting the solves. This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 9.4.
SUNLinSolSolve	`ier = SUNLinSolSolve(LS, A, x, b, tol);` Solves a linear system $Ax = b$. This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 9.4. **Direct solvers:** can ignore the `realtype` argument `tol`. **Iterative solvers:** can ignore the SUNMATRIX input `A` since a `NULL` argument will be passed (these should instead rely on the matrix-vector product function supplied through the routine `SUNLinSolSetATimes`). These should attempt to solve to the specified `realtype` tolerance `tol` in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm. **Custom solvers:** all arguments will be supplied, and if the solver is approximate then it should attempt to solve to the specified `realtype` tolerance `tol` in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.
SUNLinSolFree	`ier = SUNLinSolFree(LS);` Frees memory allocated by the linear solver. This should return zero for a successful call, and a negative value for a failure.
SUNLinSolSetATimes	`ier = SUNLinSolSetATimes(LS, A_data, ATimes);` (Iterative/Custom linear solvers only) Provides `ATimesFn` function pointer, as well as a `void *` pointer to a data structure used by this routine, to a linear solver object. SUNDIALS solvers will call this function to set the matrix-vector product function to either a solver-provided difference-quotient via vector operations or a user-supplied solver-specific routine. This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.4.

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Name	Usage and Description
SUNLinSolSetPreconditioner	`ier = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);` (Optional; Iterative/Custom linear solvers only) Provides `PSetupFn` and `PSolveFn` function pointers that implement the preconditioner solves P_1^{-1} and P_2^{-1} from equations (9.1)-(9.2). This routine will be called by a SUNDIALS solver, which will provide translation between the generic `Pset` and `Psol` calls and the integrator-specific and integrator- or user-supplied routines. This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.4.
SUNLinSolSetScalingVectors	`ier = SUNLinSolSetScalingVectors(LS, s1, s2);` (Optional; Iterative/Custom linear solvers only) Sets pointers to left/right scaling vectors for the linear system solve. Here, `s1` is an NVECTOR of positive scale factors containing the diagonal of the matrix S_1 from equations (9.1)-(9.2). Similarly, `s2` is an NVECTOR containing the diagonal of S_2 from equations (9.1)-(9.2). Neither of these vectors are tested for positivity, and a `NULL` argument for either indicates that the corresponding scaling matrix is the identity. This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.4.
SUNLinSolNumIters	`its = SUNLinSolNumIters(LS);` (Optional; Iterative/Custom linear solvers only) Should return the `int` number of linear iterations performed in the last 'solve' call.
SUNLinSolResNorm	`rnorm = SUNLinSolResNorm(LS);` (Optional; Iterative/Custom linear solvers only) Should return the `realtype` final residual norm from the last 'solve' call.
SUNLinSolResid	`rvec = SUNLinSolResid(LS);` (Optional; Iterative/Custom linear solvers only) If an iterative method computes the preconditioned initial residual and returns with a successful solve without performing any iterations (i.e. either the initial guess or the preconditioner is sufficiently accurate), then this function may be called by the SUNDIALS solver. This routine should return the NVECTOR containing the preconditioned initial residual vector.

continued on next page

Name	Usage and Description
SUNLinLastFlag	`lflag = SUNLinLastFlag(LS);` (Optional) Should return the last error flag encountered within the linear solver. This is not called by the SUNDIALS solvers directly; it allows the user to investigate linear solver issues after a failed solve.
SUNLinSolSpace	`ier = SUNLinSolSpace(LS, &lrw, &liw);` (Optional) Returns the storage requirements for the linear solver `LS`. `lrw` is a `long int` containing the number of realtype words and `liw` is a `long int` containing the number of integer words. The return value is an integer flag denoting success/failure of the operation. This function is advisory only, for use in determining a user's total space requirements.

9.0.1 Description of the client-supplied SUNLinearSolver routines

The SUNDIALS packages provide the `ATimes`, `Pset` and `Psol` routines utilized by the SUNLINSOL modules. These function types are defined in the header file `sundials/sundials_iterative.h`, and are described here in case a user wishes to interact directly with an iterative SUNLINSOL object.

`ATimesFn`

Definition `typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);`

Purpose These functions compute the action of a matrix on a vector, performing the operation $z = Av$. Memory for `z` should already be allocted prior to calling this function. The vector `v` should be left unchanged.

Arguments `A_data` is a pointer to client data, the same as that supplied to `SUNLinSolSetATimes`.
`v` is the input vector to multiply.
`z` is the output vector computed.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

Notes

`PSetupFn`

Definition `typedef int (*PSetupFn)(void *P_data)`

Purpose These functions set up any requisite problem data in preparation for calls to the corresponding `PSolveFn`.

Arguments `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

Notes

`PSolveFn`

Definition
```
typedef int (*PSolveFn)(void *P_data, N_Vector r, N_Vector z,
                        realtype tol, int lr)
```

Purpose These functions solve the preconditioner equation $Pz = r$ for the vector z. Memory for `z` should already be allocted prior to calling this function. The parameter `P_data` is a pointer to any information about P which the function needs in order to do its job (set up by the corresponding `PSetupFn`. The parameter `lr` is input, and indicates whether P is to be taken as the left preconditioner or the right preconditioner: `lr` $= 1$ for left and `lr` $= 2$ for right. If preconditioning is on one side only, `lr` can be ignored. If the preconditioner is iterative, then it should strive to solve the preconditioner equation so that

$$\|Pz - r\|_{\text{wrms}} < tol$$

where the weight vector for the WRMS norm may be accessed from the main package memory structure. The vector `r` should not be modified by the `PSolveFn`.

Arguments `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

`r` is the right-hand side vector for the preconditioner system

`z` is the solution vector for the preconditioner system

`tol` is the desired tolerance for an iterative preconditioner

`lr` is flag indicating whether the routine should perform left (1) or right (2) preconditioning.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful. On a failure, a negative return value indicates an unrecoverable condition, while a positive value indicates a recoverable one, in which the calling routine may reattempt the solution after updating preconditioner data.

Notes

9.0.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 9.3 we show the direct linear solvers available as SUNLINSOL modules, and the compatible matrix implementations. Recall that Table 4.1 shows the compatibility between all SUNLINSOL modules and vector implementations.

Table 9.3: SUNDIALS direct linear solvers and matrix implementations that can be used for each.

Linear Solver Interface	Dense Matrix	Banded Matrix	Sparse Matrix	User Supplied
Dense	✓			✓
Band		✓		✓
LapackDense	✓			✓
LapackBand		✓		✓
KLU			✓	✓
SUPERLUMT			✓	✓
User supplied	✓	✓	✓	✓

The functions within the SUNDIALS-provided `SUNLinearSolver` implementations return a common set of error codes, shown below in the Table 9.4.

Table 9.4: Description of the SUNLinearSolver error codes

Name	Value	Description
SUNLS_SUCCESS	0	successful call or converged solve
SUNLS_MEM_NULL	-1	the memory argument to the function is NULL
SUNLS_ILL_INPUT	-2	an illegal input has been provided to the function
SUNLS_MEM_FAIL	-3	failed memory access or allocation
SUNLS_ATIMES_FAIL_UNREC	-4	an unrecoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_UNREC	-5	an unrecoverable failure occurred in the Pset routine
SUNLS_PSOLVE_FAIL_UNREC	-6	an unrecoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_UNREC	-7	an unrecoverable failure occurred in an external linear solver package
SUNLS_GS_FAIL	-8	a failure occurred during Gram-Schmidt orthogonalization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_QRSOL_FAIL	-9	a singular R matrix was encountered in a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_RES_REDUCED	1	an iterative solver reduced the residual, but did not converge to the desired tolerance
SUNLS_CONV_FAIL	2	an iterative solver did not converge (and the residual was not reduced)
SUNLS_ATIMES_FAIL_REC	3	a recoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_REC	4	a recoverable failure occurred in the Pset routine
SUNLS_PSOLVE_FAIL_REC	5	a recoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_REC	6	a recoverable failure occurred in an external linear solver package
SUNLS_QRFACT_FAIL	7	a singular matrix was encountered during a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)

continued on next page

Name	Value	Description
SUNLS_LUFACT_FAIL	8	a singular matrix was encountered during a LU factorization (SUNLINSOL_DENSE/SUNLINSOL_BAND)

9.1 The SUNLinearSolver_Dense implementation

The dense implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_DENSE, is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP or NVECTOR_PTHREADS). The SUNLINSOL_DENSE module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Dense {
  sunindextype N;
  sunindextype *pivots;
  long int last_flag;
};
```

These entries of the *content* field contain the following information:

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

The header file to be included when using this module is `sunlinsol/sunlinsol_dense.h`.
The SUNLINSOL_DENSE module defines dense implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_Dense`
- `SUNLinSolInitialize_Dense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_Dense` – this performs the LU factorization.
- `SUNLinSolSolve_Dense` – this uses the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_Dense`
- `SUNLinSolSpace_Dense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_Dense`

The module SUNLINSOL_DENSE provides the following additional user-callable constructor routine:

- `SUNDenseLinearSolver`

  This function creates and allocates memory for a dense `SUNLinearSolver`. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

  If either `A` or `y` are incompatible then this routine will return `NULL`.

  ```
  SUNLinearSolver SUNDenseLinearSolver(N_Vector y, SUNMatrix A);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_DENSE module also includes the Fortran-callable function `FSUNDenseLinSolInit(code, ier)` to initialize this SUNLINSOL_DENSE module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassDenseLinSolInit(ier)` initializes this SUNLINSOL_DENSE module for solving mass matrix linear systems.

9.2 The SUNLinearSolver_Band implementation

The band implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_BAND, is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP or NVECTOR_PTHREADS). The SUNLINSOL_BAND module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Band {
  sunindextype N;
  sunindextype *pivots;
  long int last_flag;
};
```

These entries of the *content* field contain the following information:

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_BAND object.

- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `ml`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1,mu+ml)`. The lower triangular factor L has lower bandwidth `ml`.

The header file to be included when using this module is `sunlinsol/sunlinsol_band.h`.
The SUNLINSOL_BAND module defines band implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_Band`
- `SUNLinSolInitialize_Band` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_Band` – this performs the LU factorization.
- `SUNLinSolSolve_Band` – this uses the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_Band`
- `SUNLinSolSpace_Band` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_Band`

The module SUNLINSOL_BAND provides the following additional user-callable constructor routine:

- `SUNBandLinearSolver`

  This function creates and allocates memory for a band `SUNLinearSolver`. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

  Additionally, this routine will verify that the input matrix `A` is allocated with appropriate upper bandwidth storage for the LU factorization.

  If either `A` or `y` are incompatible then this routine will return `NULL`.

  ```
  SUNLinearSolver SUNBandLinearSolver(N_Vector y, SUNMatrix A);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_BAND module also includes the Fortran-callable function `FSUNBandLinSolInit(code, ier)` to initialize this SUNLINSOL_BAND module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassBandLinSolInit(ier)` initializes this SUNLINSOL_BAND module for solving mass matrix linear systems.

9.3 The SUNLinearSolver_LapackDense implementation

The LAPACK dense implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_LAPACKDENSE, is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). The SUNLINSOL_LAPACKDENSE module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Dense {
  sunindextype N;
  sunindextype *pivots;
  long int last_flag;
};
```

These entries of the *content* field contain the following information:

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

The SUNLINSOL_LAPACKDENSE module is a SUNLINSOL wrapper for the LAPACK dense matrix factorization and solve routines, `*GETRF` and `*GETRS`, where `*` is either `D` or `S`, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKDENSE module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKDENSE module also cannot be compiled when using `int64_t` for the `sunindextype`.

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

The header file to be included when using this module is `sunlinsol/sunlinsol_lapackdense.h`. The SUNLINSOL_LAPACKDENSE module defines dense implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_LapackDense`
- `SUNLinSolInitialize_LapackDense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_LapackDense` – this calls either `DGETRF` or `SGETRF` to perform the LU factorization.
- `SUNLinSolSolve_LapackDense` – this calls either `DGETRS` or `SGETRS` to use the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_LapackDense`
- `SUNLinSolSpace_LapackDense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_LapackDense`

The module SUNLINSOL_LAPACKDENSE provides the following additional user-callable constructor routine:

- `SUNLapackDense`

  This function creates and allocates memory for a LAPACK dense `SUNLinearSolver`. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_DENSE matrix

type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

If either `A` or `y` are incompatible then this routine will return `NULL`.

```
SUNLinearSolver SUNLapackDense(N_Vector y, SUNMatrix A);
```

For solvers that include a Fortran interface module, the SUNLINSOL_LAPACKDENSE module also includes the Fortran-callable function `FSUNLapackDenseInit(code, ier)` to initialize this SUNLINSOL_LAPACKDENSE module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassLapackDenseInit(ier)` initializes this SUNLINSOL_LAPACKDENSE module for solving mass matrix linear systems.

9.4 The SUNLinearSolver_LapackBand implementation

The LAPACK band implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_LAPACKBAND, is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). The SUNLINSOL_LAPACKBAND module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Band {
  sunindextype N;
  sunindextype *pivots;
  long int last_flag;
};
```

These entries of the *content* field contain the following information:

N - size of the linear system,

pivots - index array for partial pivoting in LU factorization,

last_flag - last error return flag from internal function evaluations.

The SUNLINSOL_LAPACKBAND module is a SUNLINSOL wrapper for the LAPACK band matrix factorization and solve routines, `*GBTRF` and `*GBTRS`, where `*` is either `D` or `S`, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKBAND module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKBAND module also cannot be compiled when using `int64_t` for the `sunindextype`.

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_BAND object.

- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `ml`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1,mu+ml)`. The lower triangular factor L has lower bandwidth `ml`.

The header file to be included when using this module is `sunlinsol/sunlinsol_lapackband.h`. The SUNLINSOL_LAPACKBAND module defines band implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_LapackBand`
- `SUNLinSolInitialize_LapackBand` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_LapackBand` – this calls either `DGBTRF` or `SGBTRF` to perform the LU factorization.
- `SUNLinSolSolve_LapackBand` – this calls either `DGBTRS` or `SGBTRS` to use the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_LapackBand`
- `SUNLinSolSpace_LapackBand` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_LapackBand`

The module SUNLINSOL_LAPACKBAND provides the following additional user-callable routine:

- `SUNLapackBand`

  This function creates and allocates memory for a LAPACK band `SUNLinearSolver`. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

  Additionally, this routine will verify that the input matrix `A` is allocated with appropriate upper bandwidth storage for the LU factorization.

  If either `A` or `y` are incompatible then this routine will return `NULL`.

  ```
  SUNLinearSolver SUNLapackBand(N_Vector y, SUNMatrix A);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_LAPACKBAND module also includes the Fortran-callable function `FSUNLapackBandInit(code, ier)` to initialize this SUNLINSOL_LAPACKBAND module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassLapackBandInit(ier)` initializes this SUNLINSOL_LAPACKBAND module for solving mass matrix linear systems.

9.5 The SUNLinearSolver_KLU implementation

The KLU implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_KLU, is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). The SUNLINSOL_KLU module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_KLU {
  long int         last_flag;
  int              first_factorize;
  sun_klu_symbolic *symbolic;
  sun_klu_numeric  *numeric;
  sun_klu_common   common;
  sunindextype     (*klu_solver)(sun_klu_symbolic*, sun_klu_numeric*,
                                 sunindextype, sunindextype,
                                 double*, sun_klu_common*);
};
```

These entries of the *content* field contain the following information:

last_flag - last error return flag from internal function evaluations,

first_factorize - flag indicating whether the factorization has ever been performed,

Symbolic - KLU storage structure for symbolic factorization components,

Numeric - KLU storage structure for numeric factorization components,

Common - storage structure for common KLU solver components,

klu_solver – pointer to the appropriate KLU solver function (depending on whether it is using a CSR or CSC sparse matrix).

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 14]. In order to use the SUNLINSOL_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to either `extended` or `single` (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available `sunindextype` options.

The KLU library has a symbolic factorization routine that computes the permutation of the linear system matrix to block triangular form and the permutations that will pre-order the diagonal blocks (the only ones that need to be factored) to reduce fill-in (using AMD, COLAMD, CHOLAMD, natural, or an ordering given by the user). Of these ordering choices, the default value in the SUNLINSOL_KLU module is the COLAMD ordering.

KLU breaks the factorization into two separate parts. The first is a symbolic factorization and the second is a numeric factorization that returns the factored matrix along with final pivot information. KLU also has a refactor routine that can be called instead of the numeric factorization. This routine will reuse the pivot information. This routine also returns diagnostic information that a user can examine to determine if numerical stability is being lost and a full numerical factorization should be done instead of the refactor.

Since the linear systems that arise within the context of SUNDIALS calculations will typically have identical sparsity patterns, the SUNLINSOL_KLU module is constructed to perform the following operations:

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.

- On subsequent calls to the "setup" routine, it calls the appropriate KLU "refactor" routine, followed by estimates of the numerical conditioning using the relevant "rcond", and if necessary "condest", routine(s). If these estimates of the condition number are larger than $\varepsilon^{-2/3}$ (where ε is the double-precision unit roundoff), then a new factorization is performed.

- The module includes the routine `SUNKLUReInit`, that can be called by the user to force a full refactorization at the next "setup" call.

- The "solve" call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The header file to be included when using this module is `sunlinsol/sunlinsol_klu.h`.
The SUNLINSOL_KLU module defines implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_KLU`

- `SUNLinSolInitialize_KLU` – this sets the `first_factorize` flag to 1, forcing both symbolic and numerical factorizations on the subsequent "setup" call.

- `SUNLinSolSetup_KLU` – this performs either a *LU* factorization or refactorization of the input matrix.

- `SUNLinSolSolve_KLU` – this calls the appropriate KLU solve routine to utilize the *LU* factors to solve the linear system.

- `SUNLinSolLastFlag_KLU`

- `SUNLinSolSpace_KLU` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the KLU documentation.

- `SUNLinSolFree_KLU`

The module SUNLINSOL_KLU provides the following additional user-callable routines:

- `SUNKLU`

  This constructor function creates and allocates memory for a SUNLINSOL_KLU object. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

  If either `A` or `y` are incompatible then this routine will return `NULL`.

  ```
  SUNLinearSolver SUNKLU(N_Vector y, SUNMatrix A);
  ```

- `SUNKLUReInit`

  This function reinitializes memory and flags for a new factorization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed or if the structure of the linear system has changed which would require a new symbolic (and numeric factorization).

  The `reinit_type` argument governs the level of reinitialization. The allowed values are:

1 The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.

2 Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the sparse matrix provided to the original constructor routine (or the previous `SUNKLUReInit` call).

This routine assumes no other changes to solver use are necessary.

The return values from this function are `SUNLS_MEM_NULL` (either `S` or `A` are `NULL`), `SUNLS_ILL_INPUT` (`A` does not have type `SUNMATRIX_SPARSE` or `reinit_type` is invalid), `SUNLS_MEM_FAIL` (reallocation of the sparse matrix failed) or `SUNLS_SUCCESS`.

```
int SUNKLUReInit(SUNLinearSolver S, SUNMatrix A,
                 sunindextype nnz, int reinit_type);
```

- `SUNKLUSetOrdering`

  This function sets the ordering used by KLU for reducing fill in the linear solve. Options for `ordering_choice` are:

  0 AMD,

  1 COLAMD, and

  2 the natural ordering.

  The default is 1 for COLAMD.

  The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid `ordering_choice`), or `SUNLS_SUCCESS`.

  ```
  int SUNKLUSetOrdering(SUNLinearSolver S, int ordering_choice);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_KLU module also includes the Fortran-callable function `FSUNKLUInit(code, ier)` to initialize this SUNLINSOL_KLU module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassKLUInit(ier)` initializes this SUNLINSOL_KLU module for solving mass matrix linear systems.

The `SUNKLUReInit` and `SUNKLUSetOrdering` routines also support Fortran interfaces for the system and mass matrix solvers:

- `FSUNKLUReInit(code, NNZ, reinit_type, ier)` – `NNZ` should be commensurate with a C `long int` and `reinit_type` should be commensurate with a C `int`
- `FSUNMassKLUReInit(NNZ, reinit_type, ier)`
- `FSUNKLUSetOrdering(code, ordering, ier)` – `ordering` should be commensurate with a C `int`
- `FSUNMassKLUSetOrdering(ordering, ier)`

9.6 The SUNLinearSolver_SuperLUMT implementation

The SUPERLUMT implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SUPERLUMT, is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). While these are compatible, it is not recommended to use a threaded vector module with SUNLINSOL_SUPERLUMT unless it is the NVECTOR_OPENMP module and the SUPERLUMT library has also been compiled with OpenMP. The SUNLINSOL_SUPERLUMT module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SuperLUMT {
  long int     last_flag;
  int          first_factorize;
  SuperMatrix  *A, *AC, *L, *U, *B;
  Gstat_t      *Gstat;
  sunindextype *perm_r, *perm_c;
  sunindextype N;
  int          num_threads;
  realtype     diag_pivot_thresh;
  int          ordering;
  superlumt_options_t *options;
};
```

These entries of the *content* field contain the following information:

last_flag - last error return flag from internal function evaluations,

first_factorize - flag indicating whether the factorization has ever been performed,

A, AC, L, U, B - `SuperMatrix` pointers used in solve,

Gstat - `GStat_t` object used in solve,

perm_r, perm_c - permutation arrays used in solve,

N - size of the linear system,

num_threads - number of OpenMP/Pthreads threads to use,

diag_pivot_thresh - threshold on diagonal pivoting,

ordering - flag for which reordering algorithm to use,

options - pointer to SUPERLUMT options structure.

The SUNLINSOL_SUPERLUMT module is a SUNLINSOL wrapper for the SUPERLUMT sparse matrix factorization and solver library written by X. Sherry Li [2, 28, 15]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step. In order to use the SUNLINSOL_SUPERLUMT interface to SUPERLUMT, it is assumed that SUPERLUMT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SUPERLUMT (see Appendix A for details). Additionally, this wrapper only supports single- and double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to `extended` (see Section 4.2). Moreover, since the SUPERLUMT library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SUPERLUMT library is installed using the same integer precision as the SUNDIALS `sunindextype` option.

The SUPERLUMT library has a symbolic factorization routine that computes the permutation of the linear system matrix to reduce fill-in on subsequent *LU* factorizations (using COLAMD, minimal

degree ordering on $A^T * A$, minimal degree ordering on $A^T + A$, or natural ordering). Of these ordering choices, the default value in the SUNLINSOL_SUPERLUMT module is the COLAMD ordering.

Since the linear systems that arise within the context of SUNDIALS calculations will typically have identical sparsity patterns, the SUNLINSOL_SUPERLUMT module is constructed to perform the following operations:

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.
- On subsequent calls to the "setup" routine, it skips the symbolic factorization, and only refactors the input matrix.
- The "solve" call performs pivoting and forward and backward substitution using the stored SUPERLUMT data structures. We note that in this solve SUPERLUMT operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The header file to be included when using this module is `sunlinsol/sunlinsol_superlumt.h`.
The SUNLINSOL_SUPERLUMT module defines implementations of all "direct" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_SuperLUMT`
- `SUNLinSolInitialize_SuperLUMT` – this sets the `first_factorize` flag to 1 and resets the internal SUPERLUMT statistics variables.
- `SUNLinSolSetup_SuperLUMT` – this performs either a LU factorization or refactorization of the input matrix.
- `SUNLinSolSolve_SuperLUMT` – this calls the appropriate SUPERLUMT solve routine to utilize the LU factors to solve the linear system.
- `SUNLinSolLastFlag_SuperLUMT`
- `SUNLinSolSpace_SuperLUMT` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SUPERLUMT documentation.
- `SUNLinSolFree_SuperLUMT`

The module SUNLINSOL_SUPERLUMT provides the following additional user-callable routines:

- `SUNSuperLUMT`

  This constructor function creates and allocates memory for a SUNLINSOL_SUPERLUMT object. Its arguments are an NVECTOR, a SUNMATRIX, and a desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps. This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SUPERLUMT library.

  This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

  If either `A` or `y` are incompatible then this routine will return `NULL`. The `num_threads` argument is not checked and is passed directly to SUPERLUMT routines.

  ```
  SUNLinearSolver SUNSuperLUMT(N_Vector y, SUNMatrix A, int num_threads);
  ```

- `SUNSuperLUMTSetOrdering`

  This function sets the ordering used by SUPERLUMT for reducing fill in the linear solve. Options for `ordering_choice` are:

0 natural ordering

1 minimal degree ordering on $A^T A$

2 minimal degree ordering on $A^T + A$

3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid `ordering_choice`), or `SUNLS_SUCCESS`.

```
int SUNSuperLUMTSetOrdering(SUNLinearSolver S, int ordering_choice);
```

For solvers that include a Fortran interface module, the SUNLINSOL_SUPERLUMT module also includes the Fortran-callable function `FSUNSuperLUMTInit(code, num_threads, ier)` to initialize this SUNLINSOL_SUPERLUMT module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `num_threads` is the desired number of OpenMP/Pthreads threads to use in the factorization; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these arguments should be declared so as to match C type `int`. This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassSuperLUMTInit(num_threads, ier)` initializes this SUNLINSOL_SUPERLUMT module for solving mass matrix linear systems.

The `SUNSuperLUMTSetOrdering` routine also supports Fortran interfaces for the system and mass matrix solvers:

- `FSUNSuperLUMTSetOrdering(code, ordering, ier)` – `ordering` should be commensurate with a C `int`
- `FSUNMassSuperLUMTSetOrdering(ordering, ier)`

9.7 The SUNLinearSolver_SPGMR implementation

The SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [33]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SPGMR, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`).

The SUNLINSOL_SPGMR module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector *V;
```

```
  realtype **Hes;
  realtype *givens;
  N_Vector xcor;
  realtype *yg;
  N_Vector vtemp;
};
```

These entries of the *content* field contain the following information:

maxl - number of GMRES basis vectors to use (default is 5),

pretype - flag for type of preconditioning to employ (default is none),

gstype - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

max_restarts - number of GMRES restarts to allow (default is 0),

numiters - number of iterations from the most-recent solve,

resnorm - final linear residual norm from the most-recent solve,

last_flag - last error return flag from an internal function,

ATimes - function pointer to perform Av product,

ATData - pointer to structure for `ATimes`,

Psetup - function pointer to preconditioner setup routine,

Psolve - function pointer to preconditioner solve routine,

PData - pointer to structure for `Psetup` and `Psolve`,

s1, s2 - vector pointers for supplied scaling matrices (default is `NULL`),

V - the array of Krylov basis vectors $v_1, \ldots, v_{\texttt{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

Hes - the $(\texttt{maxl}+1) \times \texttt{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`.,

givens - a length `2*maxl` array which represents the Givens rotation matrices that arise in the GMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where $F_i = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c_i & -s_i & & \\ & & & s_i & c_i & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{bmatrix}$, are represented in the `givens` vector as `givens[0]` $= c_0$, `givens[1]` $= s_0$, `givens[2]` $= c_1$, `givens[3]` $= s_1$, ... `givens[2j]` $= c_j$, `givens[2j+1]` $= s_j$.,

xcor - a vector which holds the scaled, preconditioned correction to the initial guess,

yg - a length `(maxl+1)` array of `realtype` values used to hold "short" vectors (e.g. y and g),

vtemp - temporary vector storage.

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the GMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

The header file to be included when using this module is `sunlinsol/sunlinsol_spgmr.h`.
The SUNLINSOL_SPGMR module defines implementations of all "iterative" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_SPGMR`
- `SUNLinSolInitialize_SPGMR`
- `SUNLinSolSetATimes_SPGMR`
- `SUNLinSolSetPreconditioner_SPGMR`
- `SUNLinSolSetScalingVectors_SPGMR`
- `SUNLinSolSetup_SPGMR`
- `SUNLinSolSolve_SPGMR`
- `SUNLinSolNumIters_SPGMR`
- `SUNLinSolResNorm_SPGMR`
- `SUNLinSolResid_SPGMR`
- `SUNLinSolLastFlag_SPGMR`
- `SUNLinSolSpace_SPGMR`
- `SUNLinSolFree_SPGMR`

The module SUNLINSOL_SPGMR provides the following additional user-callable routines:

- `SUNSPGMR`

  This constructor function creates and allocates memory for a SPGMR `SUNLinearSolver`. Its arguments are an NVECTOR, the desired type of preconditioning, and the number of Krylov basis vectors to use.

  This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If `y` is incompatible, then this routine will return `NULL`.

  A `maxl` argument that is ≤ 0 will result in the default value (5).

  Allowable inputs for `pretype` are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3); any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others

with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPGMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

```
SUNLinearSolver SUNSPGMR(N_Vector y, int pretype, int maxl);
```

- `SUNSPGMRSetPrecType`

  This function updates the type of preconditioning to use. Supported values are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3).

  This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

  ```
  int SUNSPGMRSetPrecType(SUNLinearSolver S, int pretype);
  ```

- `SUNSPGMRSetGSType`

  This function sets the type of Gram-Schmidt orthogonalization to use. Supported values are `MODIFIED_GS` (1) and `CLASSICAL_GS` (2). Any other integer input will result in a failure, returning error code `SUNLS_ILL_INPUT`.

  This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `gstype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

  ```
  int SUNSPGMRSetGSType(SUNLinearSolver S, int gstype);
  ```

- `SUNSPGMRSetMaxRestarts`

  This function sets the number of GMRES restarts to allow. A negative input will result in the default of 0.

  This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

  ```
  int SUNSPGMRSetMaxRestarts(SUNLinearSolver S, int maxrs);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_SPGMR module also includes the Fortran-callable function `FSUNSPGMRInit(code, pretype, maxl, ier)` to initialize this SUNLINSOL_SPGMR module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `pretype` and `maxl` are the same as for the C function `SUNSPGMR`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the NVECTOR object has been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassSPGMRInit(pretype, maxl, ier)` initializes this SUNLINSOL_SPGMR module for solving mass matrix linear systems.

The `SUNSPGMRSetPrecType`, `SUNSPGMRSetGSType` and `SUNSPGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPGMRSetGSType(code, gstype, ier)`
- `FSUNMassSPGMRSetGSType(gstype, ier)`
- `FSUNSPGMRSetPrecType(code, pretype, ier)`
- `FSUNMassSPGMRSetPrecType(pretype, ier)`
- `FSUNSPGMRSetMaxRS(code, maxrs, ier)`
- `FSUNMassSPGMRSetMaxRS(maxrs, ier)`

9.8 The SUNLinearSolver_SPFGMR implementation

The SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [32]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SPFGMR, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). Unlike the other Krylov iterative linear solvers supplied with SUNDIALS, FGMRES is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

The SUNLINSOL_SPFGMR module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPFGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector *V;
  N_Vector *Z;
  realtype **Hes;
  realtype *givens;
  N_Vector xcor;
  realtype *yg;
  N_Vector vtemp;
};
```

These entries of the *content* field contain the following information:

maxl - number of FGMRES basis vectors to use (default is 5),

pretype - flag for use of preconditioning (default is none),

gstype - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

max_restarts - number of FGMRES restarts to allow (default is 0),

numiters - number of iterations from the most-recent solve,

resnorm - final linear residual norm from the most-recent solve,

last_flag - last error return flag from an internal function,

ATimes - function pointer to perform Av product,

ATData - pointer to structure for `ATimes`,

Psetup - function pointer to preconditioner setup routine,

Psolve - function pointer to preconditioner solve routine,

PData - pointer to structure for `Psetup` and `Psolve`,

s1, s2 - vector pointers for supplied scaling matrices (default is `NULL`),

V - the array of Krylov basis vectors $v_1, \ldots, v_{\texttt{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

Z - the array of preconditioned Krylov basis vectors $z_1, \ldots, z_{\texttt{maxl}+1}$, stored in `Z[0]`, ..., `Z[maxl]`. Each z_i is a vector of type NVECTOR.,

Hes - the $(\texttt{maxl}+1) \times \texttt{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`.,

givens - a length `2*maxl` array which represents the Givens rotation matrices that arise in the FGMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where $F_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & -s_i & & & \\ & & & s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}$, are represented in the `givens` vector as `givens[0]` $= c_0$, `givens[1]` $= s_0$, `givens[2]` $= c_1$, `givens[3]` $= s_1$, ... `givens[2j]` $= c_j$, `givens[2j+1]` $= s_j$.,

xcor - a vector which holds the scaled, preconditioned correction to the initial guess,

yg - a length `(maxl+1)` array of `realtype` values used to hold "short" vectors (e.g. y and g),

vtemp - temporary vector storage.

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPFGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

The header file to be included when using this module is `sunlinsol/sunlinsol_spfgmr.h`.
The SUNLINSOL_SPFGMR module defines implementations of all "iterative" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_SPFGMR`
- `SUNLinSolInitialize_SPFGMR`
- `SUNLinSolSetATimes_SPFGMR`

- SUNLinSolSetPreconditioner_SPFGMR
- SUNLinSolSetScalingVectors_SPFGMR
- SUNLinSolSetup_SPFGMR
- SUNLinSolSolve_SPFGMR
- SUNLinSolNumIters_SPFGMR
- SUNLinSolResNorm_SPFGMR
- SUNLinSolResid_SPFGMR
- SUNLinSolLastFlag_SPFGMR
- SUNLinSolSpace_SPFGMR
- SUNLinSolFree_SPFGMR

The module SUNLINSOL_SPFGMR provides the following additional user-callable routines:

- SUNSPFGMR

  This constructor function creates and allocates memory for a SPFGMR SUNLinearSolver. Its arguments are an NVECTOR, a flag indicating to use preconditioning, and the number of Krylov basis vectors to use.

  This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

  A maxl argument that is ≤ 0 will result in the default value (5).

  Since the FGMRES algorithm is designed to only support right preconditioning, then any of the pretype inputs PREC_LEFT (1), PREC_RIGHT (2), or PREC_BOTH (3) will result in use of PREC_RIGHT; any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS). While it is possible to use a right-preconditioned SUNLINSOL_SPFGMR object for these packages, this use mode is not supported and may result in inferior performance.

  ```
  SUNLinearSolver SUNSPFGMR(N_Vector y, int pretype, int maxl);
  ```

- SUNSPFGMRSetPrecType

  This function updates the flag indicating use of preconditioning. Since the FGMRES algorithm is designed to only support right preconditioning, then any of the pretype inputs PREC_LEFT (1), PREC_RIGHT (2), or PREC_BOTH (3) will result in use of PREC_RIGHT; any other integer input will result in the default (no preconditioning).

  This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

  ```
  int SUNSPFGMRSetPrecType(SUNLinearSolver S, int pretype);
  ```

- SUNSPFGMRSetGSType

  This function sets the type of Gram-Schmidt orthogonalization to use. Supported values are MODIFIED_GS (1) and CLASSICAL_GS (2). Any other integer input will result in a failure, returning error code SUNLS_ILL_INPUT.

  This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal gstype), SUNLS_MEM_NULL (S is NULL), or SUNLS_SUCCESS.

  ```
  int SUNSPFGMRSetGSType(SUNLinearSolver S, int gstype);
  ```

- SUNSPFGMRSetMaxRestarts

  This function sets the number of FGMRES restarts to allow. A negative input will result in the default of 0.

  This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

  ```
  int SUNSPFGMRSetMaxRestarts(SUNLinearSolver S, int maxrs);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_SPFGMR module also includes the Fortran-callable function FSUNSPFGMRInit(code, pretype, maxl, ier) to initialize this SUNLINSOL_SPFGMR module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); pretype and maxl are the same as for the C function SUNSPFGMR; ier is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type int. This routine must be called *after* the NVECTOR object has been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function FSUNMassSPFGMRInit(pretype, maxl, ier) initializes this SUNLINSOL_SPFGMR module for solving mass matrix linear systems.

The SUNSPFGMRSetPrecType, SUNSPFGMRSetGSType, and SUNSPFGMRSetMaxRestarts routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C int):

- FSUNSPFGMRSetGSType(code, gstype, ier)
- FSUNMassSPFGMRSetGSType(gstype, ier)
- FSUNSPFGMRSetPrecType(code, pretype, ier)
- FSUNMassSPFGMRSetPrecType(pretype, ier)
- FSUNSPFGMRSetMaxRS(code, maxrs, ier)
- FSUNMassSPFGMRSetMaxRS(maxrs, ier)

9.9 The SUNLinearSolver_SPBCGS implementation

The SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [36]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SPBCGS, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (N_VClone, N_VDotProd, N_VScale, N_VLinearSum, N_VProd, N_VDiv, and N_VDestroy). Unlike the SPGMR and SPFGMR algorithms, SPBCGS requires a fixed amount of memory that does not increase with the number of allowed iterations.

The SUNLINSOL_SPBCGS module defines the *content* field of a SUNLinearSolver to be the following structure:

```
struct _SUNLinearSolverContent_SPBCGS {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
```

```
  N_Vector r;
  N_Vector r_star;
  N_Vector p;
  N_Vector q;
  N_Vector u;
  N_Vector Ap;
  N_Vector vtemp;
};
```

These entries of the *content* field contain the following information:

maxl - number of SPBCGS iterations to allow (default is 5),

pretype - flag for type of preconditioning to employ (default is none),

numiters - number of iterations from the most-recent solve,

resnorm - final linear residual norm from the most-recent solve,

last_flag - last error return flag from an internal function,

ATimes - function pointer to perform Av product,

ATData - pointer to structure for `ATimes`,

Psetup - function pointer to preconditioner setup routine,

Psolve - function pointer to preconditioner solve routine,

PData - pointer to structure for `Psetup` and `Psolve`,

s1, s2 - vector pointers for supplied scaling matrices (default is `NULL`),

r - a NVECTOR which holds the current scaled, preconditioned linear system residual,

r_star - a NVECTOR which holds the initial scaled, preconditioned linear system residual,

p, q, u, Ap, vtemp - NVECTORs used for workspace by the SPBCGS algorithm.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPBCGS to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the SPBCGS iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The header file to be included when using this module is `sunlinsol/sunlinsol_spbcgs.h`.
The SUNLINSOL_SPBCGS module defines implementations of all "iterative" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_SPBCGS`

- SUNLinSolInitialize_SPBCGS
- SUNLinSolSetATimes_SPBCGS
- SUNLinSolSetPreconditioner_SPBCGS
- SUNLinSolSetScalingVectors_SPBCGS
- SUNLinSolSetup_SPBCGS
- SUNLinSolSolve_SPBCGS
- SUNLinSolNumIters_SPBCGS
- SUNLinSolResNorm_SPBCGS
- SUNLinSolResid_SPBCGS
- SUNLinSolLastFlag_SPBCGS
- SUNLinSolSpace_SPBCGS
- SUNLinSolFree_SPBCGS

The module SUNLINSOL_SPBCGS provides the following additional user-callable routines:

- SUNSPBCGS

  This constructor function creates and allocates memory for a SPBCGS SUNLinearSolver. Its arguments are an NVECTOR, the desired type of preconditioning, and the number of linear iterations to allow.

  This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

  A maxl argument that is ≤ 0 will result in the default value (5).

  Allowable inputs for pretype are PREC_NONE (0), PREC_LEFT (1), PREC_RIGHT (2) and PREC_BOTH (3); any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPBCGS object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

  ```
  SUNLinearSolver SUNSPBCGS(N_Vector y, int pretype, int maxl);
  ```

- SUNSPBCGSSetPrecType

  This function updates the type of preconditioning to use. Supported values are PREC_NONE (0), PREC_LEFT (1), PREC_RIGHT (2), and PREC_BOTH (3).

  This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal pretype), SUNLS_MEM_NULL (S is NULL), or SUNLS_SUCCESS.

  ```
  int SUNSPBCGSSetPrecType(SUNLinearSolver S, int pretype);
  ```

- SUNSPBCGSSetMaxl

  This function updates the number of linear solver iterations to allow.

  A maxl argument that is ≤ 0 will result in the default value (5).

  This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

  ```
  int SUNSPBCGSSetMaxl(SUNLinearSolver S, int maxl);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_SPBCGS module also includes the Fortran-callable function `FSUNSPBCGSInit(code, pretype, maxl, ier)` to initialize this SUNLINSOL_SPBCGS module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `pretype` and `maxl` are the same as for the C function `SUNSPBCGS`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the NVECTOR object has been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassSPBCGSInit(pretype, maxl, ier)` initializes this SUNLINSOL_SPBCGS module for solving mass matrix linear systems.

The `SUNSPBCGSSetPrecType` and `SUNSPBCGSSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPBCGSSetPrecType(code, pretype, ier)`
- `FSUNMassSPBCGSSetPrecType(pretype, ier)`
- `FSUNSPBCGSSetMaxl(code, maxl, ier)`
- `FSUNMassSPBCGSSetMaxl(maxl, ier)`

9.10 The SUNLinearSolver_SPTFQMR implementation

The SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [17]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SPTFQMR, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, SPTFQMR requires a fixed amount of memory that does not increase with the number of allowed iterations.

The SUNLINSOL_SPTFQMR module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPTFQMR {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector r_star;
  N_Vector q;
  N_Vector d;
  N_Vector v;
  N_Vector p;
  N_Vector *r;
  N_Vector u;
  N_Vector vtemp1;
  N_Vector vtemp2;
  N_Vector vtemp3;
};
```

These entries of the *content* field contain the following information:

maxl - number of TFQMR iterations to allow (default is 5),

pretype - flag for type of preconditioning to employ (default is none),

numiters - number of iterations from the most-recent solve,

resnorm - final linear residual norm from the most-recent solve,

last_flag - last error return flag from an internal function,

ATimes - function pointer to perform Av product,

ATData - pointer to structure for `ATimes`,

Psetup - function pointer to preconditioner setup routine,

Psolve - function pointer to preconditioner solve routine,

PData - pointer to structure for `Psetup` and `Psolve`,

s1, s2 - vector pointers for supplied scaling matrices (default is `NULL`),

r_star - a NVECTOR which holds the initial scaled, preconditioned linear system residual,

q, d, v, p, u - NVECTORs used for workspace by the SPTFQMR algorithm,

r - array of two NVECTORs used for workspace within the SPTFQMR algorithm,

vtemp1, vtemp2, vtemp3 - temporary vector storage.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPTFQMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the TFQMR iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The header file to be included when using this module is `sunlinsol/sunlinsol_sptfqmr.h`.
The SUNLINSOL_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_SPTFQMR`
- `SUNLinSolInitialize_SPTFQMR`
- `SUNLinSolSetATimes_SPTFQMR`
- `SUNLinSolSetPreconditioner_SPTFQMR`
- `SUNLinSolSetScalingVectors_SPTFQMR`

- SUNLinSolSetup_SPTFQMR
- SUNLinSolSolve_SPTFQMR
- SUNLinSolNumIters_SPTFQMR
- SUNLinSolResNorm_SPTFQMR
- SUNLinSolResid_SPTFQMR
- SUNLinSolLastFlag_SPTFQMR
- SUNLinSolSpace_SPTFQMR
- SUNLinSolFree_SPTFQMR

The module SUNLINSOL_SPTFQMR provides the following additional user-callable routines:

- SUNSPTFQMR

  This constructor function creates and allocates memory for a SPTFQMR SUNLinearSolver. Its arguments are an NVECTOR, the desired type of preconditioning, and the number of linear iterations to allow.

  This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

  A maxl argument that is ≤ 0 will result in the default value (5).

  Allowable inputs for pretype are PREC_NONE (0), PREC_LEFT (1), PREC_RIGHT (2) and PREC_BOTH (3); any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPTFQMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

  ```
  SUNLinearSolver SUNSPTFQMR(N_Vector y, int pretype, int maxl);
  ```

- SUNSPTFQMRSetPrecType

  This function updates the type of preconditioning to use. Supported values are PREC_NONE (0), PREC_LEFT (1), PREC_RIGHT (2), and PREC_BOTH (3).

  This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal pretype), SUNLS_MEM_NULL (S is NULL), or SUNLS_SUCCESS.

  ```
  int SUNSPTFQMRSetPrecType(SUNLinearSolver S, int pretype);
  ```

- SUNSPTFQMRSetMaxl

  This function updates the number of linear solver iterations to allow.

  A maxl argument that is ≤ 0 will result in the default value (5).

  This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

  ```
  int SUNSPTFQMRSetMaxl(SUNLinearSolver S, int maxl);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_SPTFQMR module also includes the Fortran-callable function FSUNSPTFQMRInit(code, pretype, maxl, ier) to initialize this SUNLINSOL_SPTFQMR module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); pretype and maxl are the same as for the C function SUNSPTFQMR; ier is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type int. This routine must be called *after* the NVECTOR object has been initialized. Additionally, when using ARKODE with a non-identity

mass matrix, the Fortran-callable function `FSUNMassSPTFQMRInit(pretype, maxl, ier)` initializes this SUNLINSOL_SPTFQMR module for solving mass matrix linear systems.

The `SUNSPTFQMRSetPrecType` and `SUNSPTFQMRSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPTFQMRSetPrecType(code, pretype, ier)`
- `FSUNMassSPTFQMRSetPrecType(pretype, ier)`
- `FSUNSPTFQMRSetMaxl(code, maxl, ier)`
- `FSUNMassSPTFQMRSetMaxl(maxl, ier)`

9.11 The SUNLinearSolver_PCG implementation

The PCG (Preconditioned Conjugate Gradient [18]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_PCG, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, PCG requires a fixed amount of memory that does not increase with the number of allowed iterations.

Unlike all of the other iterative linear solvers supplied with SUNDIALS, PCG should only be used on *symmetric* linear systems (e.g. mass matrix linear systems encountered in ARKODE). As a result, the explanation of the role of scaling and preconditioning matrices given in general must be modified in this scenario. The PCG algorithm solves a linear system $Ax = b$ where A is a symmetric ($A^T = A$), real-valued matrix. Preconditioning is allowed, and is applied in a symmetric fashion on both the right and left. Scaling is also allowed and is applied symmetrically. We denote the preconditioner and scaling matrices as follows:

- P is the preconditioner (assumed symmetric),
- S is a diagonal matrix of scale factors.

The matrices A and P are not required explicitly; only routines that provide A and P^{-1} as operators are required. The diagonal of the matrix S is held in a single NVECTOR, supplied by the user.

In this notation, PCG applies the underlying CG algorithm to the equivalent transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.3}$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \tag{9.4}$$

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

$$\begin{aligned} & \|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta \\ \Leftrightarrow \\ & \|SP^{-1}b - SP^{-1}Ax\|_2 < \delta \\ \Leftrightarrow \\ & \|P^{-1}b - P^{-1}Ax\|_S < \delta \end{aligned}$$

where $\|v\|_S = \sqrt{v^T S^T S v}$, with an input tolerance δ.

The SUNLINSOL_PCG module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_PCG {
  int maxl;
  int pretype;
  int numiters;
  realtype resnorm;
  long int last_flag;
  ATimesFn ATimes;
  void* ATData;
  PSetupFn Psetup;
  PSolveFn Psolve;
  void* PData;
  N_Vector s;
  N_Vector r;
  N_Vector p;
  N_Vector z;
  N_Vector Ap;
};
```

These entries of the *content* field contain the following information:

maxl - number of PCG iterations to allow (default is 5),

pretype - flag for use of preconditioning (default is none),

numiters - number of iterations from the most-recent solve,

resnorm - final linear residual norm from the most-recent solve,

last_flag - last error return flag from an internal function,

ATimes - function pointer to perform Av product,

ATData - pointer to structure for `ATimes`,

Psetup - function pointer to preconditioner setup routine,

Psolve - function pointer to preconditioner solve routine,

PData - pointer to structure for `Psetup` and `Psolve`,

s - vector pointer for supplied scaling matrix (default is `NULL`),

r - a NVECTOR which holds the preconditioned linear system residual,

p, z, Ap - NVECTORs used for workspace by the PCG algorithm.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_PCG to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s` scaling vector.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The header file to be included when using this module is `sunlinsol/sunlinsol_pcg.h`.
The SUNLINSOL_PCG module defines implementations of all "iterative" linear solver operations listed in Table 9.2:

- `SUNLinSolGetType_PCG`
- `SUNLinSolInitialize_PCG`
- `SUNLinSolSetATimes_PCG`
- `SUNLinSolSetPreconditioner_PCG`
- `SUNLinSolSetScalingVectors_PCG` – since PCG only supports symmetric scaling, the second NVECTOR argument to this function is ignored
- `SUNLinSolSetup_PCG`
- `SUNLinSolSolve_PCG`
- `SUNLinSolNumIters_PCG`
- `SUNLinSolResNorm_PCG`
- `SUNLinSolResid_PCG`
- `SUNLinSolLastFlag_PCG`
- `SUNLinSolSpace_PCG`
- `SUNLinSolFree_PCG`

The module SUNLINSOL_PCG provides the following additional user-callable routines:

- `SUNPCG`

  This constructor function creates and allocates memory for a PCG `SUNLinearSolver`. Its arguments are an NVECTOR, a flag indicating to use preconditioning, and the number of linear iterations to allow.

  This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If `y` is incompatible then this routine will return `NULL`.

  A `maxl` argument that is ≤ 0 will result in the default value (5).

  Since the PCG algorithm is designed to only support symmetric preconditioning, then any of the `pretype` inputs `PREC_LEFT` (1), `PREC_RIGHT` (2), or `PREC_BOTH` (3) will result in use of the symmetric preconditioner; any other integer input will result in the default (no preconditioning). Although some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL), PCG should *only* be used with these packages when the linear systems are known to be *symmetric*. Since the scaling of matrix rows and columns must be identical in a symmetric matrix, symmetric preconditioning should work appropriately even for packages designed with one-sided preconditioning in mind.

  ```
  SUNLinearSolver SUNPCG(N_Vector y, int pretype, int maxl);
  ```

- `SUNPCGSetPrecType`

  This function updates the flag indicating use of preconditioning. As above, any one of the input values, `PREC_LEFT` (1), `PREC_RIGHT` (2), or `PREC_BOTH` (3) will enable preconditioning; `PREC_NONE` (0) disables preconditioning.

This routine will return with one of the error codes SUNLS_ILL_INPUT (illegal pretype), SUNLS_MEM_NULL (S is NULL), or SUNLS_SUCCESS.

```
int SUNPCGSetPrecType(SUNLinearSolver S, int pretype);
```

- SUNPCGSetMaxl

  This function updates the number of linear solver iterations to allow.

  A maxl argument that is ≤ 0 will result in the default value (5).

  This routine will return with one of the error codes SUNLS_MEM_NULL (S is NULL) or SUNLS_SUCCESS.

  ```
  int SUNPCGSetMaxl(SUNLinearSolver S, int maxl);
  ```

For solvers that include a Fortran interface module, the SUNLINSOL_PCG module also includes the Fortran-callable function FSUNPCGInit(code, pretype, maxl, ier) to initialize this SUNLINSOL_PCG module for a given SUNDIALS solver. Here code is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); pretype and maxl are the same as for the C function SUNPCG; ier is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type int. This routine must be called *after* the NVECTOR object has been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function FSUNMassPCGInit(pretype, maxl, ier) initializes this SUNLINSOL_PCG module for solving mass matrix linear systems.

The SUNPCGSetPrecType and SUNPCGSetMaxl routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C int):

- FSUNPCGSetPrecType(code, pretype, ier)
- FSUNMassPCGSetPrecType(pretype, ier)
- FSUNPCGSetMaxl(code, maxl, ier)
- FSUNMassPCGSetMaxl(maxl, ier)

9.12 SUNLinearSolver Examples

There are SUNLinearSolver examples that may be installed for each implementation; these make use of the functions in test_sunlinsol.c. These example functions show simple usage of the SUNLinearSolver family of functions. The inputs to the examples depend on the linear solver type, and are output to stdout if the example is run without the appropriate number of command-line arguments.
The following is a list of the example functions in test_sunlinsol.c:

- Test_SUNLinSolGetType: Verifies the returned solver type against the value that should be returned.
- Test_SUNLinSolInitialize: Verifies that SUNLinSolInitialize can be called and returns successfully.
- Test_SUNLinSolSetup: Verifies that SUNLinSolSetup can be called and returns successfully.
- Test_SUNLinSolSolve: Given a SUNMATRIX object A, NVECTOR objects x and b (where $Ax = b$) and a desired solution tolerance tol, this routine clones x into a new vector y, calls SUNLinSolSolve to fill y as the solution to $Ay = b$ (to the input tolerance), verifies that each entry in x and y match to within 10*tol, and overwrites x with y prior to returning (in case the calling routine would like to investigate further).
- Test_SUNLinSolSetATimes (iterative solvers only): Verifies that SUNLinSolSetATimes can be called and returns successfully.

- `Test_SUNLinSolSetPreconditioner` (iterative solvers only): Verifies that `SUNLinSolSetPreconditioner` can be called and returns successfully.
- `Test_SUNLinSolSetScalingVectors` (iterative solvers only): Verifies that `SUNLinSolSetScalingVectors` can be called and returns successfully.
- `Test_SUNLinSolLastFlag`: Verifies that `SUNLinSolLastFlag` can be called, and outputs the result to `stdout`.
- `Test_SUNLinSolNumIters` (iterative solvers only): Verifies that `SUNLinSolNumIters` can be called, and outputs the result to `stdout`.
- `Test_SUNLinSolResNorm` (iterative solvers only): Verifies that `SUNLinSolResNorm` can be called, and that the result is non-negative.
- `Test_SUNLinSolResid` (iterative solvers only): Verifies that `SUNLinSolResid` can be called.
- `Test_SUNLinSolSpace` verifies that `SUNLinSolSpace` can be called, and outputs the results to `stdout`.

We'll note that these tests should be performed in a particular order. For either direct or iterative linear solvers, `Test_SUNLinSolInitialize` must be called before `Test_SUNLinSolSetup`, which must be called before `Test_SUNLinSolSolve`. Additionally, for iterative linear solvers `Test_SUNLinSolSetATimes`, `Test_SUNLinSolSetPreconditioner` and `Test_SUNLinSolSetScalingVectors` should be called before `Test_SUNLinSolInitialize`; similarly `Test_SUNLinSolNumIters`, `Test_SUNLinSolResNorm` and `Test_SUNLinSolResid` should be called after `Test_SUNLinSolSolve`. These are called in the appropriate order in all of the example problems.

9.13 SUNLinearSolver functions used by IDAS

In Table 9.5 below, we list the linear solver functions in the SUNLINSOL module used within the IDAS package. The table also shows, for each function, which of the code modules uses the function. In general, the main IDAS integrator considers three categories of linear solvers, *direct*, *iterative* and *custom*, with interfaces accessible in the IDAS header files `idas_direct.h` (IDADLS), `idas_spils.h` (IDASPILS) and `idas_customls.h` (IDACLS), respectively. Hence, the the table columns reference the use of SUNLINSOL functions by each of these solver interfaces.

As with the SUNMATRIX module, we emphasize that the IDAS user does not need to know detailed usage of linear solver functions by the IDAS code modules in order to use IDAS. The information is presented as an implementation detail for the interested reader.

The linear solver functions listed in Table 9.2 with a † symbol are optionally used, in that these are only called if they are implemented in the SUNLINSOL module that is being used (i.e. their function pointers are non-`NULL`). Also, although IDAS does not call the `SUNLinSolLastFlag` or `SUNLinSolFree` routines directly, these are available for users to query linear solver issues and free linear solver memory directly.

Table 9.5: List of linear solver functions usage by IDAS code modules

	IDADLS	IDASPILS	IDACLS
SUNLinSolGetType	✓	✓	†
SUNLinSolSetATimes		✓	†
SUNLinSolSetPreconditioner		✓	†
SUNLinSolSetScalingVectors		✓	†
SUNLinSolInitialize	✓	✓	✓
SUNLinSolSetup	✓	✓	✓
SUNLinSolSolve	✓	✓	✓
SUNLinSolNumIters		✓	†
SUNLinSolResNorm		✓	†
SUNLinSolResid		✓	†
SUNLinSolLastFlag			
SUNLinSolFree			
SUNLinSolSpace	†	†	†

Chapter 10

Providing Alternate Linear Solver Modules

The central IDAS module interfaces with a linear solver module by way of calls to five functions. These are denoted here by `linit`, `lsetup`, `lsolve`, `lperf`, and `lfree`. Briefly, their purposes are as follows:

- `linit`: initialize memory specific to the linear solver;
- `lsetup`: evaluate and preprocess the Jacobian or preconditioner;
- `lsolve`: solve the linear system;
- `lperf`: monitor performance and issue warnings;
- `lfree`: free the linear solver memory.

A linear solver module must also provide a user-callable **specification function** (like those described in §4.5.3) which will attach the above five functions to the main IDAS memory block. The IDAS memory block is a structure defined in the header file `idas_impl.h`. A pointer to such a structure is defined as the type `IDAMem`. The five fields in an `IDAMem` structure that must point to the linear solver's functions are `ida_linit`, `ida_lsetup`, `ida_lsolve`, `ida_lperf`, and `ida_lfree`, respectively. Note that of the five interface functions, only `lsolve` is required. The `lfree` function must be provided only if the solver specification function makes any memory allocation. For any of the functions that are *not* provided, the corresponding field should be set to `NULL`. The linear solver specification function must also set the value of the field `ida_setupNonNull` in the IDAS memory block — to `TRUE` if `lsetup` is used, or `FALSE` otherwise.

Typically, the linear solver will require a block of memory specific to the solver, and a principal function of the specification function is to allocate that memory block, and initialize it. Then the field `ida_lmem` in the IDAS memory block is available to attach a pointer to that linear solver memory. This block can then be used to facilitate the exchange of data between the five interface functions.

If the linear solver involves adjustable parameters, the specification function should set the default values of those. User-callable functions may be defined that could, optionally, override the default parameter values.

We encourage the use of performance counters in connection with the various operations involved with the linear solver. Such counters would be members of the linear solver memory block, would be initialized in the `linit` function, and would be incremented by the `lsetup` and `lsolve` functions. Then, user-callable functions would be needed to obtain the values of these counters.

For consistency with the existing IDAS linear solver modules, we recommend that the return value of the specification function be 0 for a successful return, and a negative value if an error occurs. Possible error conditions include: the pointer to the main IDAS memory block is `NULL`, an input is illegal, the NVECTOR implementation is not compatible, or a memory allocation fails.

To be used during the backward integration with the IDAS module, a linear solver module must also provide an additional user-callable specification function (like those described in §6.2.6) which will attach the five functions to the IDAS memory block for each backward integration. Note that this block, of type `IDAMem`, is not directly accessible to the specification function, but rather is itself a field in the IDAS memory block. For a given backward problem identifier `which`, the corresponding memory block must be located in the linked list starting at `ida_mem->ida_adj_mem->IDAB_mem`; see for example the function `IDADenseB` for specific details. This specification function must also allocate the linear solver memory for the backward problem, and attach that, as well as a corresponding memory free function, to the above block `IDAB_mem`, of type `struct IDABMemRec`. The specification function for backward integration should return a negative value if it encounters an illegal input, if backward integration has not been initialized, or if its memory allocation failed.

These five functions, which interface between IDAS and the linear solver module, necessarily have fixed call sequences. Thus a user wishing to implement another linear solver within the IDAS package must adhere to this set of interfaces. The following is a complete description of the call list for each of these functions. Note that the call list of each function includes a pointer to the main IDAS memory block, by which the function can access various data related to the IDAS solution. The contents of this memory block are given in the file `idas_impl.h` (but not reproduced here, for the sake of space).

10.1 Initialization function

The type definition of `linit` is

`linit`

Definition `int (*linit)(IDAMem IDA_mem);`

Purpose The purpose of `linit` is to complete initializations for the specific linear solver, such as counters and statistics. It should also set pointers to data blocks that will later be passed to functions associated with the linear solver. The `linit` function is called once only, at the start of the problem, during the first call to `IDASolve`.

Arguments `IDA_mem` is the IDAS memory pointer of type `IDAMem`.

Return value An `linit` function should return 0 if it has successfully initialized the IDAS linear solver and a negative value otherwise.

10.2 Setup function

The type definition of `lsetup` is

`lsetup`

Definition
```
int (*lsetup)(IDAMem IDA_mem, N_Vector yyp, N_Vector ypp, N_Vector resp,
              N_Vector vtemp1, N_Vector vtemp2, N_Vector vtemp3);
```

Purpose The job of `lsetup` is to prepare the linear solver for subsequent calls to `lsolve`, in the solution of systems $Mx = b$, where M is some approximation to the system Jacobian, $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$. (See Eqn. (2.6), in which $\alpha = cj$). Here cj is available as `IDA_mem->ida_cj`.

The `lsetup` function may call a user-supplied function, or a function within the linear solver module, to compute Jacobian-related data that is required by the linear solver. It may also preprocess that data as needed for `lsolve`, which may involve calling a generic function (such as for LU factorization). This data may be intended either for direct use (in a direct linear solver) or for use in a preconditioner (in a preconditioned iterative linear solver).

The `lsetup` function is not called at every time step, but only as frequently as the solver determines that it is appropriate to perform the setup task. In this way, Jacobian-related data generated by `lsetup` is expected to be used over a number of time steps.

Arguments
- `IDA_mem` is the IDAS memory pointer of type `IDAMem`.
- `yyp` is the predicted y vector for the current IDAS internal step.
- `ypp` is the predicted $\dot{y}$ vector for the current IDAS internal step.
- `resp` is the value of the residual function at `yyp` and `ypp`, i.e. $F(t_n, y_{pred}, \dot{y}_{pred})$.
- `vtemp1`
- `vtemp2`
- `vtemp3` are temporary variables of type `N_Vector` provided for use by `lsetup`.

Return value The `lsetup` function should return 0 if successful, a positive value for a recoverable error, and a negative value for an unrecoverable error. On a recoverable error return, the solver will attempt to recover by reducing the step size.

10.3 Solve function

The type definition of `lsolve` is

`lsolve`

Definition
```
int (*lsolve)(IDAMem IDA_mem, N_Vector b, N_Vector weight,
              N_Vector ycur, N_Vector ypcur, N_Vector rescur);
```

Purpose The `lsolve` function must solve the linear system, $Mx = b$, where M is some approximation to the system Jacobian, $J = \partial F/\partial y + cj\, \partial F/\partial \dot{y}$ (see Eqn. (2.6), in which $\alpha = cj$), and the right-hand side vector, b, is input. Here cj is available as `IDA_mem->ida_cj`.

`lsolve` is called once per Newton iteration, hence possibly several times per time step.

If there is an `lsetup` function, this `lsolve` function should make use of any Jacobian data that was computed and preprocessed by `lsetup`, either for direct use, or for use in a preconditioner.

Arguments
- `IDA_mem` is the IDAS memory pointer of type `IDAMem`.
- `b` is the right-hand side vector b. The solution is to be returned in the vector `b`.
- `weight` is a vector that contains the error weights. These are the W_i of (2.7). This weight vector is included here to enable the computation of weighted norms needed to test for the convergence of iterative methods (if any) within the linear solver.
- `ycur` is a vector that contains the solver's current approximation to $y(t_n)$.
- `ypcur` is a vector that contains the solver's current approximation to $\dot{y}(t_n)$.
- `rescur` is a vector that contains the current residual, $F(t_n$, `ycur`, `ypcur`$)$.

Return value The `lsolve` function should return a positive value for a recoverable error and a negative value for an unrecoverable error. Success is indicated by a 0 return value. On a recoverable error return, the solver will attempt to recover, such as by calling the `lsetup` function with current arguments.

10.4 Performance monitoring function

The type definition of `lperf` is

`lperf`

Definition `int (*lperf)(IDAMem IDA_mem, int perftask);`

Purpose The `lperf` function is to monitor the performance of the linear solver. It can be used to compute performance metrics related to the linear solver and issue warnings if these indicate poor performance of the linear solver. The `lperf` function is called with `perftask` = 0 at the start of each call to `IDASolve`, and then is called with `perftask` = 1 just before each internal time step.

Arguments `IDA_mem` is the IDAS memory pointer of type `IDAMem`.

`perftask` is a task flag. `perftask` = 0 means initialize needed counters. `perftask` = 1 means evaluate performance and issue warnings if needed. Counters that are used to compute performance metrics (e.g. counts of iterations within the `lsolve` function) should be initialized here when `perftask` = 0, and used for the calculation of metrics when `perftask` = 1.

Return value The `lperf` return value is ignored.

10.5 Memory deallocation function

The type definition of `lfree` is

`lfree`

Definition `int (*lfree)(IDAMem IDA_mem);`

Purpose The `lfree` function should free up any memory allocated by the linear solver.

Arguments The argument `IDA_mem` is the IDAS memory pointer of type `IDAMem`.

Return value The `lfree` function should return 0 if successful, or a nonzero if not.

Notes This function is called once a problem has been completed and the linear solver is no longer needed.

Chapter 11

General Use Linear Solver Components in SUNDIALS

In this chapter, we describe linear solver code components that are included in SUNDIALS, but which are of potential use as generic packages in themselves, either in conjunction with the use of SUNDIALS or separately.

These generic modules in SUNDIALS are organized in three families, the *dls* family, which includes direct linear solvers appropriate for sequential computations; the *sls* family, which includes sparse matrix solvers; and the *spils* family, which includes scaled preconditioned iterative (Krylov) linear solvers. The solvers in each family share common data structures and functions.

The *dls* family contains the following two generic linear solvers:

- The DENSE package, a linear solver for dense matrices either specified through a matrix type (defined below) or as simple arrays.
- The BAND package, a linear solver for banded matrices either specified through a matrix type (defined below) or as simple arrays.

Note that this family also includes the Blas/Lapack linear solvers (dense and band) available to the SUNDIALS solvers, but these are not discussed here.

The *sls* family contains a sparse matrix package and interfaces between it and two sparse direct solver packages:

- The KLU package, a linear solver for compressed-sparse-column matrices, [1, 14].
- The SUPERLUMT package, a threaded linear solver for compressed-sparse-column matrices, [2, 28, 15].

The *spils* family contains the following generic linear solvers:

- The SPGMR package, a solver for the scaled preconditioned GMRES method.
- The SPFGMR package, a solver for the scaled preconditioned Flexible GMRES method.
- The SPBCGS package, a solver for the scaled preconditioned Bi-CGStab method.
- The SPTFQMR package, a solver for the scaled preconditioned TFQMR method.

For reasons related to installation, the names of the files involved in these packages begin with the prefix `sundials_`. But despite this, each of the *dls* and *spils* solvers is in fact generic, in that it is usable completely independently of SUNDIALS.

For the sake of space, the functions for the `dense` and `band` modules that work with a matrix type, and the functions in the SPGMR, SPFGMR, SPBCGS, and SPTFQMR modules are only summarized briefly, since they are less likely to be of direct use in connection with a SUNDIALS solver. However, the

functions for dense matrices treated as simple arrays and sparse matrices are fully described, because we expect that they will be useful in the implementation of preconditioners used with the combination of one of the SUNDIALS solvers and one of the *spils* linear solvers.

11.1 The DLS modules: DENSE and BAND

The files comprising the DENSE generic linear solver, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir*/include/sundials)
  sundials_direct.h, sundials_dense.h,
  sundials_types.h, sundials_math.h, sundials_config.h
- source files (located in *srcdir*/src/sundials)
  sundials_direct.c, sundials_dense.c, sundials_math.c

The files comprising the BAND generic linear solver are as follows:

- header files (located in *srcdir*/include/sundials)
  sundials_direct.h, sundials_band.h,
  sundials_types.h, sundials_math.h, sundials_config.h
- source files (located in *srcdir*/src/sundials)
  sundials_direct.c, sundials_band.c, sundials_math.c

Only two of the preprocessing directives in the header file sundials_config.h are relevant to the DENSE and BAND packages by themselves.

- (required) definition of the precision of the SUNDIALS type realtype. One of the following lines must be present:
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
- (optional) use of generic math functions: #define SUNDIALS_USE_GENERIC_MATH 1

The sundials_types.h header file defines the SUNDIALS realtype and booleantype types and the macro RCONST, while the sundials_math.h header file is needed for the macros SUNMIN and SUNMAX, and the function SUNRabs.

The files listed above for either module can be extracted from the SUNDIALS *srcdir* and compiled by themselves into a separate library or into a larger user code.

11.1.1 Type DlsMat

The type DlsMat, defined in sundials_direct.h is a pointer to a structure defining a generic matrix, and is used with all linear solvers in the *dls* family:

```
typedef struct _DlsMat {
  int type;
  sunindextype M;
  sunindextype N;
  sunindextype ldim;
  sunindextype mu;
  sunindextype ml;
  sunindextype s_mu;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
} *DlsMat;
```

For the DENSE module, the relevant fields of this structure are as follows. Note that a dense matrix of type `DlsMat` need not be square.

type - `SUNDIALS_DENSE` (=1)

M - number of rows

N - number of columns

ldim - leading dimension (`ldim` $\geq$ `M`)

data - pointer to a contiguous block of `realtype` variables

ldata - length of the data array (= `ldim`·`N`). The (`i`,`j`)-th element of a dense matrix `A` of type `DlsMat` (with 0 $\leq$ `i` $<$ `M` and 0 $\leq$ `j` $<$ `N`) is given by the expression `(A->data)[0][j*M+i]`

cols - array of pointers. `cols[j]` points to the first element of the j-th column of the matrix in the array data. The (`i`,`j`)-th element of a dense matrix `A` of type `DlsMat` (with 0 $\leq$ `i` $<$ `M` and 0 $\leq$ `j` $<$ `N`) is given by the expression `(A->cols)[j][i]`

For the BAND module, the relevant fields of this structure are as follows (see Figure 11.1 for a diagram of the underlying data representation in a banded matrix of type `DlsMat`). Note that only square band matrices are allowed.

type - `SUNDIALS_BAND` (=2)

M - number of rows

N - number of columns (`N` = `M`)

mu - upper half-bandwidth, 0 $\leq$ `mu` $<$ min(`M`,`N`)

ml - lower half-bandwidth, 0 $\leq$ `ml` $<$ min(`M`,`N`)

s_mu - storage upper bandwidth, `mu` $\leq$ `s_mu` $<$ `N`. The LU decomposition routine writes the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(`N`-1,`mu`+`ml`) because of partial pivoting. The `s_mu` field holds the upper half-bandwidth allocated for A.

ldim - leading dimension (`ldim` $\geq$ `s_mu`)

data - pointer to a contiguous block of `realtype` variables. The elements of a banded matrix of type `DlsMat` are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. `data` is a pointer to `ldata` contiguous locations which hold the elements within the band of A.

ldata - length of the data array (= `ldim`·(`s_mu`+`ml`+1)

cols - array of pointers. `cols[j]` is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from `s_mu`−`mu` (to access the uppermost element within the band in the j-th column) to `s_mu`+`ml` (to access the lowest element within the band in the j-th column). Indices from 0 to `s_mu`−`mu`−1 give access to extra storage elements required by the LU decomposition function. Finally, `cols[j][i-j+s_mu]` is the (i, j)-th element, j−`mu` $\leq i \leq j$+`ml`.

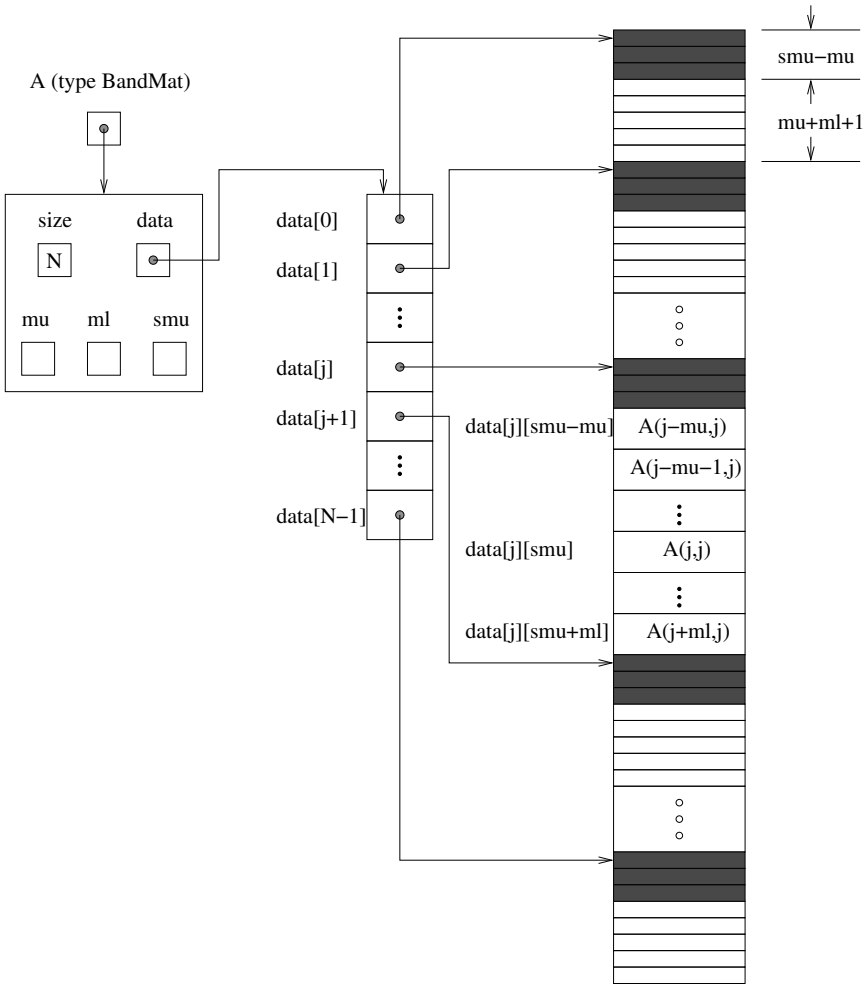

Figure 11.1: Diagram of the storage for a banded matrix of type `DlsMat`. Here `A` is an $N \times N$ band matrix of type `DlsMat` with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to $N-1$ and the (i,j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the `BandGBTRF` and `BandGBTRS` routines.

11.1.2 Accessor macros for the DLS modules

The macros below allow a user to efficiently access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer to the j-th column of elements can be obtained via the DENSE_COL or BAND_COL macros. Users should use these macros whenever possible.

The following two macros are defined by the DENSE module to provide access to data in the DlsMat type:

- DENSE_ELEM

  Usage : DENSE_ELEM(A,i,j) = a_ij; or a_ij = DENSE_ELEM(A,i,j);

  DENSE_ELEM references the (i,j)-th element of the $M \times N$ DlsMat A, $0 \le$ i $< M$, $0 \le$ j $< N$.

- DENSE_COL

  Usage : col_j = DENSE_COL(A,j);

  DENSE_COL references the j-th column of the $M \times N$ DlsMat A, $0 \le$ j $< N$. The type of the expression DENSE_COL(A,j) is realtype * . After the assignment in the usage above, col_j may be treated as an array indexed from 0 to $M - 1$. The (i, j)-th element of A is referenced by col_j[i].

The following three macros are defined by the BAND module to provide access to data in the DlsMat type:

- BAND_ELEM

  Usage : BAND_ELEM(A,i,j) = a_ij; or a_ij = BAND_ELEM(A,i,j);

  BAND_ELEM references the (i,j)-th element of the $N \times N$ band matrix A, where $0 \le$ i, j $\le N - 1$. The location (i,j) should further satisfy j−(A->mu) $\le$ i $\le$ j+(A->ml).

- BAND_COL

  Usage : col_j = BAND_COL(A,j);

  BAND_COL references the diagonal element of the j-th column of the $N \times N$ band matrix A, $0 \le$ j $\le N - 1$. The type of the expression BAND_COL(A,j) is realtype *. The pointer returned by the call BAND_COL(A,j) can be treated as an array which is indexed from −(A->mu) to (A->ml).

- BAND_COL_ELEM

  Usage : BAND_COL_ELEM(col_j,i,j) = a_ij; or a_ij = BAND_COL_ELEM(col_j,i,j);

  This macro references the (i,j)-th entry of the band matrix A when used in conjunction with BAND_COL to reference the j-th column through col_j. The index (i,j) should satisfy j−(A->mu) $\le$ i $\le$ j+(A->ml).

11.1.3 Functions in the DENSE module

The DENSE module defines two sets of functions with corresponding names. The first set contains functions (with names starting with a capital letter) that act on dense matrices of type DlsMat. The second set contains functions (with names starting with a lower case letter) that act on matrices represented as simple arrays.

The following functions for DlsMat dense matrices are available in the DENSE package. For full details, see the header files sundials_direct.h and sundials_dense.h.

- NewDenseMat: allocation of a DlsMat dense matrix;
- DestroyMat: free memory for a DlsMat matrix;

- `PrintMat`: print a `DlsMat` matrix to standard output.
- `NewIndexArray`: allocation of an array of integers for use as pivots with `DenseGETRF` and `DenseGETRS`;
- `NewIntArray`: allocation of an array of `int` integers for use as pivots with the Lapack dense solvers;
- `NewRealArray`: allocation of an array of `realtype` for use as right-hand side with `DenseGETRS`;
- `DestroyArray`: free memory for an array;
- `SetToZero`: load a matrix with zeros;
- `AddIdentity`: increment a square matrix by the identity matrix;
- `DenseCopy`: copy one matrix to another;
- `DenseScale`: scale a matrix by a scalar;
- `DenseGETRF`: LU factorization with partial pivoting;
- `DenseGETRS`: solution of $Ax = b$ using LU factorization (for square matrices A);
- `DensePOTRF`: Cholesky factorization of a real symmetric positive matrix;
- `DensePOTRS`: solution of $Ax = b$ using the Cholesky factorization of A;
- `DenseGEQRF`: QR factorization of an $m \times n$ matrix, with $m \geq n$;
- `DenseORMQR`: compute the product $w = Qv$, with Q calculated using `DenseGEQRF`;
- `DenseMatvec`: compute the product $y = Ax$, for an M by N matrix A;

The following functions for small dense matrices are available in the DENSE package:

- `newDenseMat`

  `newDenseMat(m,n)` allocates storage for an `m` by `n` dense matrix. It returns a pointer to the newly allocated storage if successful. If the memory request cannot be satisfied, then `newDenseMat` returns `NULL`. The underlying type of the dense matrix returned is `realtype**`. If we allocate a dense matrix `realtype** a` by `a = newDenseMat(m,n)`, then `a[j][i]` references the (`i`,`j`)-th element of the matrix `a`, $0 \leq$ `i` $<$ `m`, $0 \leq$ `j` $< n$, and `a[j]` is a pointer to the first element in the `j`-th column of `a`. The location `a[0]` contains a pointer to `m` $\times$ `n` contiguous locations which contain the elements of `a`.

- `destroyMat`

  `destroyMat(a)` frees the dense matrix `a` allocated by `newDenseMat`;

- `newIndexArray`

  `newIndexArray(n)` allocates an array of `n` integers, all `sunindextype`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `newIntArray`

  `newIntArray(n)` allocates an array of `n` integers, all `int`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `newRealArray`

  `newRealArray(n)` allocates an array of `n realtype` values. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `destroyArray`

  `destroyArray(p)` frees the array `p` allocated by `newIndexArray`, `newIntArray`, or `newRealArray`;

- `denseCopy`

  `denseCopy(a,b,m,n)` copies the `m` by `n` dense matrix `a` into the `m` by `n` dense matrix `b`;

- `denseScale`

  `denseScale(c,a,m,n)` scales every element in the `m` by `n` dense matrix `a` by the scalar `c`;

- `denseAddIdentity`

  `denseAddIdentity(a,n)` increments the *square* `n` by `n` dense matrix `a` by the identity matrix I_n;

- `denseGETRF`

  `denseGETRF(a,m,n,p)` factors the `m` by `n` dense matrix `a`, using Gaussian elimination with row pivoting. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.

  A successful LU factorization leaves the matrix `a` and the pivot array `p` with the following information:

  1. `p[k]` contains the row number of the pivot element chosen at the beginning of elimination step `k`, `k` $= 0, 1, ...,$`n`-1.
  2. If the unique LU factorization of `a` is given by $Pa = LU$, where P is a permutation matrix, L is an `m` by `n` lower trapezoidal matrix with all diagonal elements equal to 1, and U is an `n` by `n` upper triangular matrix, then the upper triangular part of `a` (including its diagonal) contains U and the strictly lower trapezoidal part of `a` contains the multipliers, $I - L$. If `a` is square, L is a unit lower triangular matrix.

     `denseGETRF` returns 0 if successful. Otherwise it encountered a zero diagonal element during the factorization, indicating that the matrix `a` does not have full column rank. In this case it returns the column index (numbered from one) at which it encountered the zero.

- `denseGETRS`

  `denseGETRS(a,n,p,b)` solves the `n` by `n` linear system $ax = b$. It assumes that `a` (of size `n` $\times$ `n`) has been LU-factored and the pivot array `p` has been set by a successful call to `denseGETRF(a,n,n,p)`. The solution x is written into the `b` array.

- `densePOTRF`

  `densePOTRF(a,m)` calculates the Cholesky decomposition of the `m` by `m` dense matrix `a`, assumed to be symmetric positive definite. Only the lower triangle of `a` is accessed and overwritten with the Cholesky factor.

- `densePOTRS`

  `densePOTRS(a,m,b)` solves the `m` by `m` linear system $ax = b$. It assumes that the Cholesky factorization of `a` has been calculated in the lower triangular part of `a` by a successful call to `densePOTRF(a,m)`.

- `denseGEQRF`

  `denseGEQRF(a,m,n,beta,wrk)` calculates the QR decomposition of the `m` by `n` matrix `a` (`m` $\geq$ `n`) using Householder reflections. On exit, the elements on and above the diagonal of `a` contain the `n` by `n` upper triangular matrix `R`; the elements below the diagonal, with the array `beta`, represent the orthogonal matrix `Q` as a product of elementary reflectors. The real array `wrk`, of length `m`, must be provided as temporary workspace.

- `denseORMQR`

  `denseORMQR(a,m,n,beta,v,w,wrk)` calculates the product $w = Qv$ for a given vector `v` of length `n`, where the orthogonal matrix Q is encoded in the `m` by `n` matrix `a` and the vector `beta` of length `n`, after a successful call to `denseGEQRF(a,m,n,beta,wrk)`. The real array `wrk`, of length `m`, must be provided as temporary workspace.

- `denseMatvec`

  `denseMatvec(a,x,y,m,n)` calculates the product $y = ax$ for a given vector `x` of length `n`, and `m` by `n` matrix `a`.

11.1.4 Functions in the BAND module

The BAND module defines two sets of functions with corresponding names. The first set contains functions (with names starting with a capital letter) that act on band matrices of type `DlsMat`. The second set contains functions (with names starting with a lower case letter) that act on matrices represented as simple arrays.

The following functions for `DlsMat` banded matrices are available in the BAND package. For full details, see the header files `sundials_direct.h` and `sundials_band.h`.

- `NewBandMat`: allocation of a `DlsMat` band matrix;
- `DestroyMat`: free memory for a `DlsMat` matrix;
- `PrintMat`: print a `DlsMat` matrix to standard output.
- `NewIndexArray`: allocation of an array of integers for use as pivots with `BandGBRF` and `BandGBRS`;
- `NewIntArray`: allocation of an array of `int` integers for use as pivots with the Lapack band solvers;
- `NewRealArray`: allocation of an array of `realtype` for use as right-hand side with `BandGBRS`;
- `DestroyArray`: free memory for an array;
- `SetToZero`: load a matrix with zeros;
- `AddIdentity`: increment a square matrix by the identity matrix;
- `BandCopy`: copy one matrix to another;
- `BandScale`: scale a matrix by a scalar;
- `BandGBTRF`: LU factorization with partial pivoting;
- `BandGBTRS`: solution of $Ax = b$ using LU factorization;
- `BandMatvec`: compute the product $y = Ax$, for a square band matrix A;

The following functions for small band matrices are available in the BAND package:

- `newBandMat`

  `newBandMat(n, smu, ml)` allocates storage for an `n` by `n` band matrix with lower half-bandwidth `ml`.

- `destroyMat`

  `destroyMat(a)` frees the band matrix `a` allocated by `newBandMat`;

- `newIndexArray`

  `newIndexArray(n)` allocates an array of `n` integers, all `sunindextype`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `newIntArray`

  `newIntArray(n)` allocates an array of `n` integers, all `int`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `newRealArray`

  `newRealArray(n)` allocates an array of `n realtype` values. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.

- `destroyArray`

  `destroyArray(p)` frees the array `p` allocated by `newIndexArray`, `newIntArray`, or `newRealArray`;

- `bandCopy`

  `bandCopy(a,b,n,a_smu, b_smu,copymu, copyml)` copies the `n` by `n` band matrix `a` into the `n` by `n` band matrix `b`;

- `bandScale`

  `bandScale(c,a,n,mu,ml,smu)` scales every element in the `n` by `n` band matrix `a` by `c`;

- `bandAddIdentity`

  `bandAddIdentity(a,n,smu)` increments the `n` by `n` band matrix `a` by the identity matrix;

- `bandGETRF`

  `bandGETRF(a,n,mu,ml,smu,p)` factors the `n` by `n` band matrix `a`, using Gaussian elimination with row pivoting. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.

- `bandGETRS`

  `bandGETRS(a,n,smu,ml,p,b)` solves the `n` by `n` linear system $ax = b$. It assumes that `a` (of size `n` $\times$ `n`) has been LU-factored and the pivot array `p` has been set by a successful call to `bandGETRF(a,n,mu,ml,smu,p)`. The solution x is written into the `b` array.

- `bandMatvec`

  `bandMatvec(a,x,y,n,mu,ml,smu)` calculates the product $y = ax$ for a given vector `x` of length `n`, and `n` by `n` band matrix `a`.

11.2 The SLS module

SUNDIALS provides a compressed-sparse-column matrix type and sparse matrix support functions. In addition, SUNDIALS provides interfaces to the publically available KLU and SuperLU_MT sparse direct solver packages. The files comprising the SLS matrix module, used in the KLU and SUPERLUMT linear solver packages, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir*`/include/sundials`)
  `sundials_sparse.h`, `sundials_klu_impl.h`,
  `sundials_superlumt_impl.h`, `sundials_types.h`,
  `sundials_math.h`, `sundials_config.h`

- source files (located in *srcdir*`/src/sundials`)
  `sundials_sparse.c`, `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are relevant to the SLS package by itself:

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```
- (optional) use of generic math functions: `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the macros `SUNMIN` and `SUNMAX`, and the function `SUNRabs`.

11.2.1 Type SlsMat

SUNDIALS supports operations with matrices either in compressed-sparse-column (CSC) format or in compressed-sparse-row (CSR) format. For convenience, integer sparse matrix identifiers are defined as:

```
#define CSC_MAT 0
#define CSR_MAT 1
```

The type `SlsMat`, defined in `sundials_sparse.h` is a pointer to a structure defining generic CSC and CSR matrix formats, and is used with all linear solvers in the *sls* family:

```
typedef struct _SlsMat {
  int M;
  int N;
  int NNZ;
  int NP;
  realtype *data;
  int sparsetype;
  int *indexvals;
  int *indexptrs;
  int **rowvals;
  int **colptrs;
  int **colvals;
  int **rowptrs;
} *SlsMat;
```

The fields of this structure are as follows (see Figure 11.2 for a diagram of the underlying compressed-sparse-column representation in a sparse matrix of type `SlsMat`). Note that a sparse matrix of type `SlsMat` need not be square.

M - number of rows

N - number of columns

NNZ - maximum number of nonzero entries in the matrix (allocated length of `data` and `rowvals` arrays)

NP - number of index pointers (e.g. number of column pointers for CSC matrix). For CSC matrices $NP = N$, and for CSR matrices $NP = M$. This value is set automatically based the input for `sparsetype`.

data - pointer to a contiguous block of `realtype` variables (of length `NNZ`), containing the values of the nonzero entries in the matrix

sparsetype - type of the sparse matrix (`CSC_MAT` or `CSR_MAT`)

indexvals - pointer to a contiguous block of `int` variables (of length `NNZ`), containing the row indices (if CSC) or column indices (if CSR) of each nonzero matrix entry held in `data`

indexptrs - pointer to a contiguous block of `int` variables (of length `NP+1`). For CSC matrices each entry provides the index of the first column entry into the `data` and `indexvals` arrays, e.g. if `indexptr[3]=7`, then the first nonzero entry in the fourth column of the matrix is located in `data[7]`, and is located in row `indexvals[7]` of the matrix. The last entry contains the total number of nonzero values in the matrix and hence points one past the end of the active data in the `data` and `indexvals` arrays. For CSR matrices, each entry provides the index of the first row entry into the `data` and `indexvals` arrays.

The following pointers are added to the `SlsMat` type for user convenience, to provide a more intuitive interface to the CSC and CSR sparse matrix data structures. They are set automatically by the `SparseNewMat` function, based on the sparse matrix storage type.

rowvals - pointer to `indexvals` when `sparsetype` is `CSC_MAT`, otherwise set to `NULL`.

colptrs - pointer to `indexptrs` when `sparsetype` is `CSC_MAT`, otherwise set to `NULL`.

colvals - pointer to `indexvals` when `sparsetype` is `CSR_MAT`, otherwise set to `NULL`.

rowptrs - pointer to `indexptrs` when `sparsetype` is `CSR_MAT`, otherwise set to `NULL`.

For example, the 5×4 CSC matrix

$$\begin{bmatrix} 0 & 3 & 1 & 0 \\ 3 & 0 & 0 & 2 \\ 0 & 7 & 0 & 0 \\ 1 & 0 & 0 & 9 \\ 0 & 0 & 0 & 5 \end{bmatrix}$$

could be stored in a `SlsMat` structure as either

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4};
indexptrs = {0, 2, 4, 5, 8};
rowvals = &indexvals;
colptrs = &indexptrs;
colvals = NULL;
rowptrs = NULL;
```

or

```
M = 5;
N = 4;
NNZ = 10;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0, *, *};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4, *, *};
indexptrs = {0, 2, 4, 5, 8};
...
```

where the first has no unused space, and the second has additional storage (the entries marked with * may contain any values). Note in both cases that the final value in indexptrs is 8. The work associated with operations on the sparse matrix is proportional to this value and so one should use the best understanding of the number of nonzeroes here.

11.2.2 Functions in the SLS module

The SLS module defines functions that act on sparse matrices of type SlsMat. For full details, see the header file sundials_sparse.h.

- SparseNewMat

  SparseNewMat(M, N, NNZ, sparsetype) allocates storage for an M by N sparse matrix, with storage for up to NNZ nonzero entries and sparsetype storage type (CSC_MAT or CSR_MAT).

- SparseFromDenseMat

  SparseFromDenseMat(A) converts a dense or band matrix A of type DlsMat into a new CSC matrix of type SlsMat by retaining only the nonzero values of the matrix A.

- SparseDestroyMat

  SparseDestroyMat(A) frees the memory for a sparse matrix A allocated by either SparseNewMat or SparseFromDenseMat.

- SparseSetMatToZero(A) zeros out the SlsMat matrix A. The storage for A is left unchanged.

- SparseCopyMat

  SparseCopyMat(A, B) copies the SlsMat A into the SlsMat B. It is assumed that the matrices have the same row/column dimensions and storage type. If B has insufficient storage to hold all the nonzero entries of A, the data and index arrays in B are reallocated to match those in A.

- SparseScaleMat

  SparseScaleMat(c, A) scales every element in the SlsMat A by the realtype scalar c.

- SparseAddIdentityMat

  SparseAddIdentityMat(A) increments the SlsMat A by the identity matrix. If A is not square, only the existing diagonal values are incremented. Resizes the data and rowvals arrays of A to allow for new nonzero entries on the diagonal.

- SparseAddMat

  SparseAddMat(A, B) adds two SlsMat matrices A and B, placing the result back in A. Resizes the data and rowvals arrays of A upon completion to exactly match the nonzero storage for the result. Upon successful completion, the return value is zero; otherwise -1 is returned. It is assumed that both matrices have the same size and storage type.

- SparseReallocMat

  SparseReallocMat(A) eliminates unused storage in the SlsMat A by resizing the internal data and rowvals arrays to contain exactly colptrs[N] values.

- SparseMatvec

  SparseMatvec(A, x, y) computes the sparse matrix-vector product, $y = Ax$. If the SlsMat A is a sparse matrix of dimension $M \times N$, then it is assumed that x is a realtype array of length N, and y is a realtype array of length M. Upon successful completion, the return value is zero; otherwise -1 is returned.

- SparsePrintMat

  SparsePrintMat(A) Prints the SlsMat matrix A to standard output.

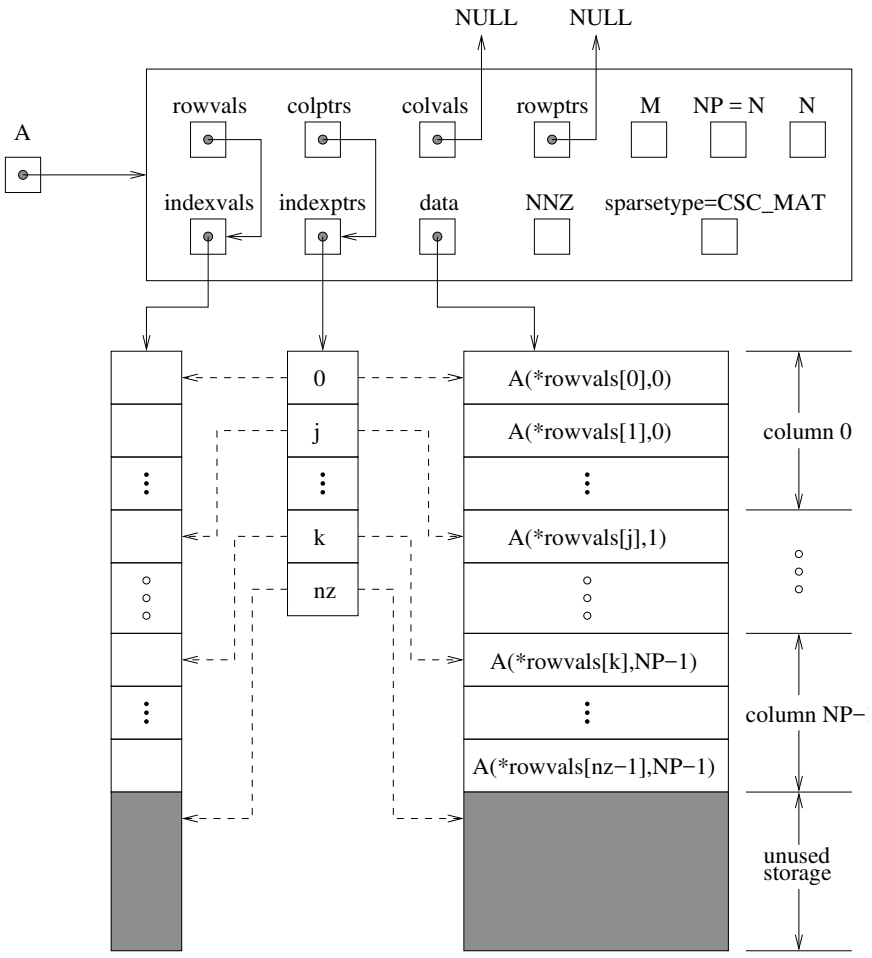

Figure 11.2: Diagram of the storage for a compressed-sparse-column matrix of type `SlsMat`. Here `A` is an $M \times N$ sparse matrix of type `SlsMat` with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to $M-1$, corresponding to the row index (zero-based) of each nonzero value. The entries in `data` contain the values of the nonzero entries, with the row i, column j entry of `A` (again, zero-based) denoted as `A(i,j)`. The `indexptrs` array contains $N+1$ entries; the first N denote the starting index of each column within the `indexvals` and `data` arrays, while the final entry points one past the final nonzero entry. Here, although `NNZ` values are allocated, only `nz` are actually filled in; the greyed-out portions of `data` and `indexvals` indicate extra allocated space.

11.2.3 The KLU solver

KLU is a sparse matrix factorization and solver library written by Tim Davis [1, 14]. KLU has a symbolic factorization routine that computes the permutation of the linear system matrix to block triangular form and the permutations that will pre-order the diagonal blocks (the only ones that need to be factored) to reduce fill-in (using AMD, COLAMD, CHOLAMD, natural, or an ordering given by the user). Note that SUNDIALS uses the COLAMD ordering by default with KLU.

KLU breaks the factorization into two separate parts. The first is a symbolic factorization and the second is a numeric factorization that returns the factored matrix along with final pivot information. KLU also has a refactor routine that can be called instead of the numeric factorization. This routine will reuse the pivot information. This routine also returns diagnostic information that a user can examine to determine if numerical stability is being lost and a full numerical factorization should be done instead of the refactor.

The KLU interface in SUNDIALS will perform the symbolic factorization once. It then calls the numerical factorization once and will call the refactor routine until estimates of the numerical conditioning suggest a new factorization should be completed. The KLU interface also has a `ReInit` routine that can be used to force a full refactorization at the next solver setup call.

In order to use the SUNDIALS interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details).

Designed for serial calculations only, KLU is supported for calculations employing SUNDIALS' serial or shared-memory parallel NVECTOR modules (see Sections 7.1, 7.3 and 7.4 for details).

11.2.4 The SUPERLUMT solver

SUPERLUMT is a threaded sparse matrix factorization and solver library written by X. Sherry Li [2, 28, 15]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step.

In order to use the SUNDIALS interface to SUPERLUMT, it is assumed that SUPERLUMT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SUPERLUMT (see Appendix A for details).

Designed for serial and threaded calculations only, SUPERLUMT is supported for calculations employing SUNDIALS' serial or shared-memory parallel NVECTOR modules (see Sections 7.1, 7.3 and 7.4 for details).

11.3 The SPILS modules: SPGMR, SPFGMR, SPBCG, and SPTFQMR

The *spils* modules contain implementations of some of the most commonly use scaled preconditioned Krylov solvers. A linear solver module from the *spils* family can be used in conjunction with any NVECTOR implementation library.

11.3.1 The SPGMR module

The SPGMR package, in the files `sundials_spgmr.h` and `sundials_spgmr.c`, includes an implementation of the scaled preconditioned GMRES method. A separate code module, implemented in `sundials_iterative.(h,c)`, contains auxiliary functions that support SPGMR, as well as the other Krylov solvers in SUNDIALS (SPFGMR, SPBCGS, and SPTFQMR). For full details, including usage instructions, see the header files `sundials_spgmr.h` and `sundials_iterative.h`.

The files comprising the SPGMR generic linear solver, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir*/include/sundials)
  sundials_spgmr.h, sundials_iterative.h, sundials_nvector.h,
  sundials_types.h, sundials_math.h, sundials_config.h
- source files (located in *srcdir*/src/sundials)
  sundials_spgmr.c, sundials_iterative.c, sundials_nvector.c

Only two of the preprocessing directives in the header file sundials_config.h are required to use the SPGMR package by itself:

- (required) definition of the precision of the SUNDIALS type realtype. One of the following lines must be present:
  ```
  #define SUNDIALS_DOUBLE_PRECISION 1
  #define SUNDIALS_SINGLE_PRECISION 1
  #define SUNDIALS_EXTENDED_PRECISION 1
  ```
- (optional) use of generic math functions:
  ```
  #define SUNDIALS_USE_GENERIC_MATH 1
  ```

The sundials_types.h header file defines the SUNDIALS realtype and booleantype types and the macro RCONST, while the sundials_math.h header file is needed for the macros SUNMIN, SUNMAX, and SUNSQR, and the functions SUNRabs and SUNRsqrt.

The generic NVECTOR files, sundials_nvector.(h,c) are needed for the definition of the generic N_Vector type and functions. The NVECTOR functions used by the SPGMR module are: N_VDotProd, N_VLinearSum, N_VScale, N_VProd, N_VDiv, N_VConst, N_VClone, N_VCloneVectorArray, N_VDestroy, and N_VDestroyVectorArray.

The nine files listed above can be extracted from the SUNDIALS *srcdir* and compiled by themselves into an SPGMR library or into a larger user code.

The following functions are available in the SPGMR package:

- SpgmrMalloc: allocation of memory for SpgmrSolve;
- SpgmrSolve: solution of $Ax = b$ by the SPGMR method;
- SpgmrFree: free memory allocated by SpgmrMalloc.

The following functions are available in the support package sundials_iterative.(h,c):

- ModifiedGS: performs modified Gram-Schmidt procedure;
- ClassicalGS: performs classical Gram-Schmidt procedure;
- QRfact: performs QR factorization of Hessenberg matrix;
- QRsol: solves a least squares problem with a Hessenberg matrix factored by QRfact.

11.3.2 The SPFGMR module

The SPFGMR package, in the files sundials_spfgmr.h and sundials_spfgmr.c, includes an implementation of the scaled preconditioned Flexible GMRES method. For full details, including usage instructions, see the file sundials_spfgmr.h.

The files needed to use the SPFGMR module by itself are the same as for the SPGMR module, but with sundials_spfgmr.(h,c) in place of sundials_spgmr.(h,c).

The following functions are available in the SPFGMR package:

- SpfgmrMalloc: allocation of memory for SpfgmrSolve;
- SpfgmrSolve: solution of $Ax = b$ by the SPFGMR method;
- SpfgmrFree: free memory allocated by SpfgmrMalloc.

11.3.3 The SPBCG module

The SPBCGS package, in the files `sundials_spbcgs.h` and `sundials_spbcgs.c`, includes an implementation of the scaled preconditioned Bi-CGStab method. For full details, including usage instructions, see the file `sundials_spbcgs.h`.

The files needed to use the SPBCGS module by itself are the same as for the SPGMR module, but with `sundials_spbcgs.(h,c)` in place of `sundials_spgmr.(h,c)`.

The following functions are available in the SPBCGS package:

- `SpbcgMalloc`: allocation of memory for `SpbcgSolve`;
- `SpbcgSolve`: solution of $Ax = b$ by the SPBCGS method;
- `SpbcgFree`: free memory allocated by `SpbcgMalloc`.

11.3.4 The SPTFQMR module

The SPTFQMR package, in the files `sundials_sptfqmr.h` and `sundials_sptfqmr.c`, includes an implementation of the scaled preconditioned TFQMR method. For full details, including usage instructions, see the file `sundials_sptfqmr.h`.

The files needed to use the SPTFQMR module by itself are the same as for the SPGMR module, but with `sundials_sptfqmr.(h,c)` in place of `sundials_spgmr.(h,c)`.

The following functions are available in the SPTFQMR package:

- `SptfqmrMalloc`: allocation of memory for `SptfqmrSolve`;
- `SptfqmrSolve`: solution of $Ax = b$ by the SPTFQMR method;
- `SptfqmrFree`: free memory allocated by `SptfqmrMalloc`.

Appendix A

SUNDIALS Package Installation Procedure

The installation of any SUNDIALS package is accomplished by installing the SUNDIALS suite as a whole, according to the instructions that follow. The same procedure applies whether or not the downloaded file contains one or all solvers in SUNDIALS.

The SUNDIALS suite (or individual solvers) are distributed as compressed archives (`.tar.gz`). The name of the distribution archive is of the form *solver*`-x.y.z.tar.gz`, where *solver* is one of: `sundials`, `cvode`, `cvodes`, `arkode`, `ida`, `idas`, or `kinsol`, and `x.y.z` represents the version number (of the SUNDIALS suite or of the individual solver) . To begin the installation, first uncompress and expand the sources, by issuing

```
% tar xzf solver-x.y.z.tar.gz
```

This will extract source files under a directory *solver*`-x.y.z`.

Starting with version `2.6.0` of SUNDIALS, CMake is the only supported method of installation. The explanations of the installation procedure begins with a few common observations:

- The remainder of this chapter will follow these conventions:

  srcdir is the directory *solver*`-x.y.z` created above; i.e., the directory containing the SUNDIALS sources.

  builddir is the (temporary) directory under which SUNDIALS is built.

  instdir is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory *instdir*`/include` while libraries are installed under *instdir*`/lib`, with *instdir* specified at configuration time.

- For SUNDIALS CMake-based installation, in-source builds are prohibited; in other words, the build directory *builddir* can **not** be the same as *srcdir* and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.

- The installation directory *instdir* can **not** be the same as the source directory *srcdir*.

- By default, only the libraries and header files are exported to the installation directory *instdir*. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the *installed* SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as "templates" for your own problems. CMake installs `CMakeLists.txt` files and also (as an option available only under Unix/Linux) `Makefile` files. Note this installation

approach also allows the option of building the SUNDIALS examples without having to install them. (This can be used as a sanity check for the freshly built libraries.)

- Even if generation of shared libraries is enabled, only static libraries are created for the FCMIX modules. (Because of the use of fixed names for the Fortran user-provided subroutines, FCMIX shared libraries would result in "undefined symbol" errors at link time.)

A.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Makefiles, as well as KDevelop, Visual Studio, and (Apple) XCode project files from the same configuration file. In addition, CMake also provides a GUI front end and which allows an interactive build and installation process.

The SUNDIALS build process requires CMake version `2.8.1` or higher and a working C compiler. On Unix-like operating systems, it also requires Make (and `curses`, including its development libraries, for the GUI front end to CMake, `ccmake`), while on Windows it requires Visual Studio. While many Linux distributions offer CMake, the version included is probably out of date. Many new CMake features have been added recently, and you should download the latest version from `http://www.cmake.org`. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use `ccmake`, while Windows users will be able to use `CMakeSetup`.

As previously noted, when using CMake to configure, build and install SUNDIALS, it is always required to use a separate build directory. While in-source builds are possible, they are explicitly prohibited by the SUNDIALS CMake scripts (one of the reasons being that, unlike autotools, CMake does not provide a `make distclean` procedure and it is therefore difficult to clean-up the source tree after an in-source build). By ensuring a separate build directory, it is an easy task for the user to clean-up all traces of the build by simply removing the build directory. CMake does generate a `make clean` which will remove files generated by the compiler and linker.

A.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The *installdir* defaults to `/usr/local` and can be changed by setting the `CMAKE_INSTALL_PREFIX` variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the `cmake` command, or from a `curses`-based GUI by using the `ccmake` command. Examples for using both methods will be presented. For the examples shown it is assumed that there is a top level SUNDIALS directory with appropriate source, build and install directories:

```
% mkdir (...)sundials/instdir
% mkdir (...)sundials/builddir
% cd (...)sundials/builddir
```

Building with the GUI

Using CMake with the GUI follows this general process:

- Select and modify values, run configure (`c` key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
  - If it is a boolean (ON/OFF) it will toggle the value
  - If it is string or file, it will allow editing of the string

  - For file and directories, the `<tab>` key can be used to complete

- Repeat until all values are set as desired and the generate option is available (`g` key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (`t` key)
- To search for a variable press `/` key, and to repeat the search, press the `n` key

To build the default configuration using the GUI, from the *builddir* enter the ccmake command and point to the *srcdir*:

```
% ccmake ../srcdir
```

The default configuration screen is shown in Figure A.1.

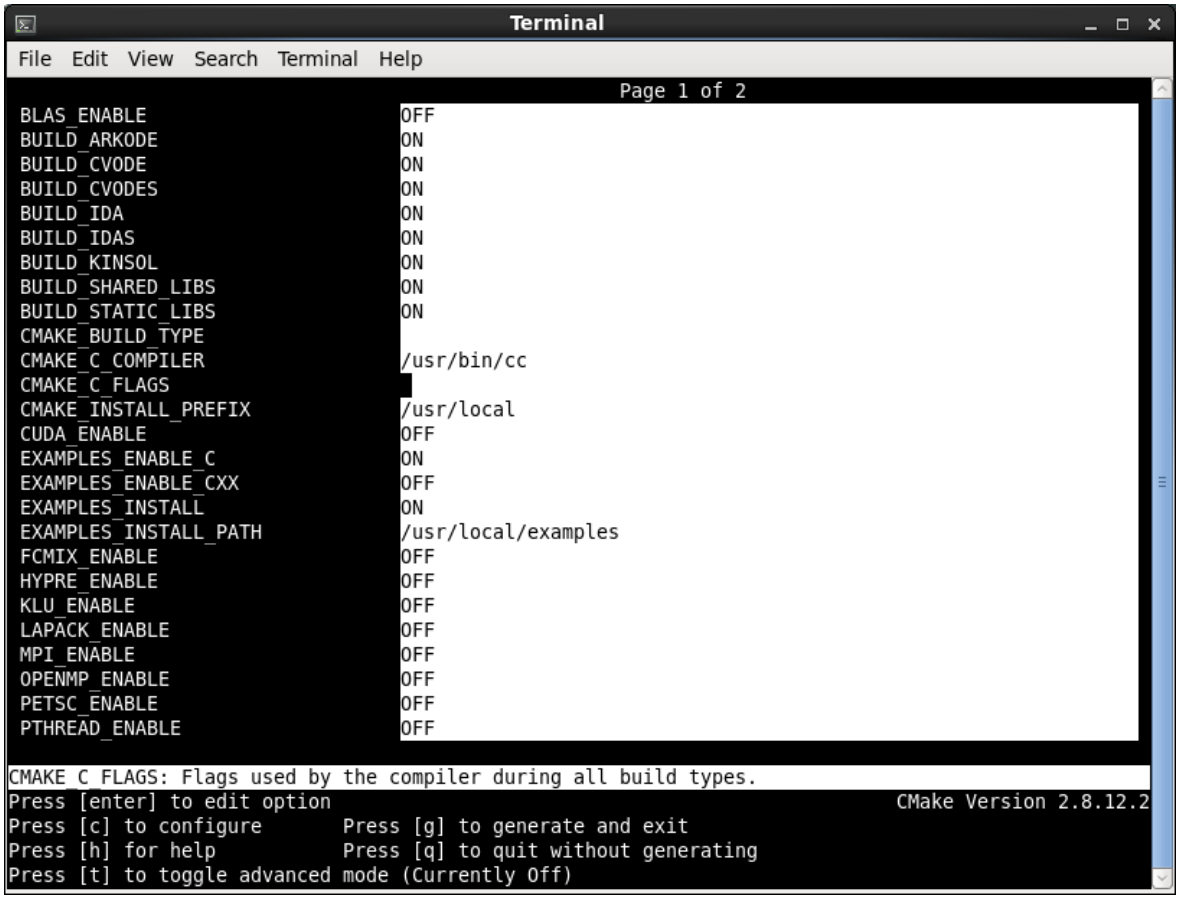

Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the `CMAKE_INSTALL_PREFIX` and the `EXAMPLES_INSTALL_PATH` as shown in figure A.2.

Pressing the (`g` key) will generate makefiles including all dependencies and all rules to build SUNDIALS on this system. Back at the command prompt, you can now run:

```
% make
```

To install SUNDIALS in the installation directory specified in the configuration, simply run:

```
% make install
```

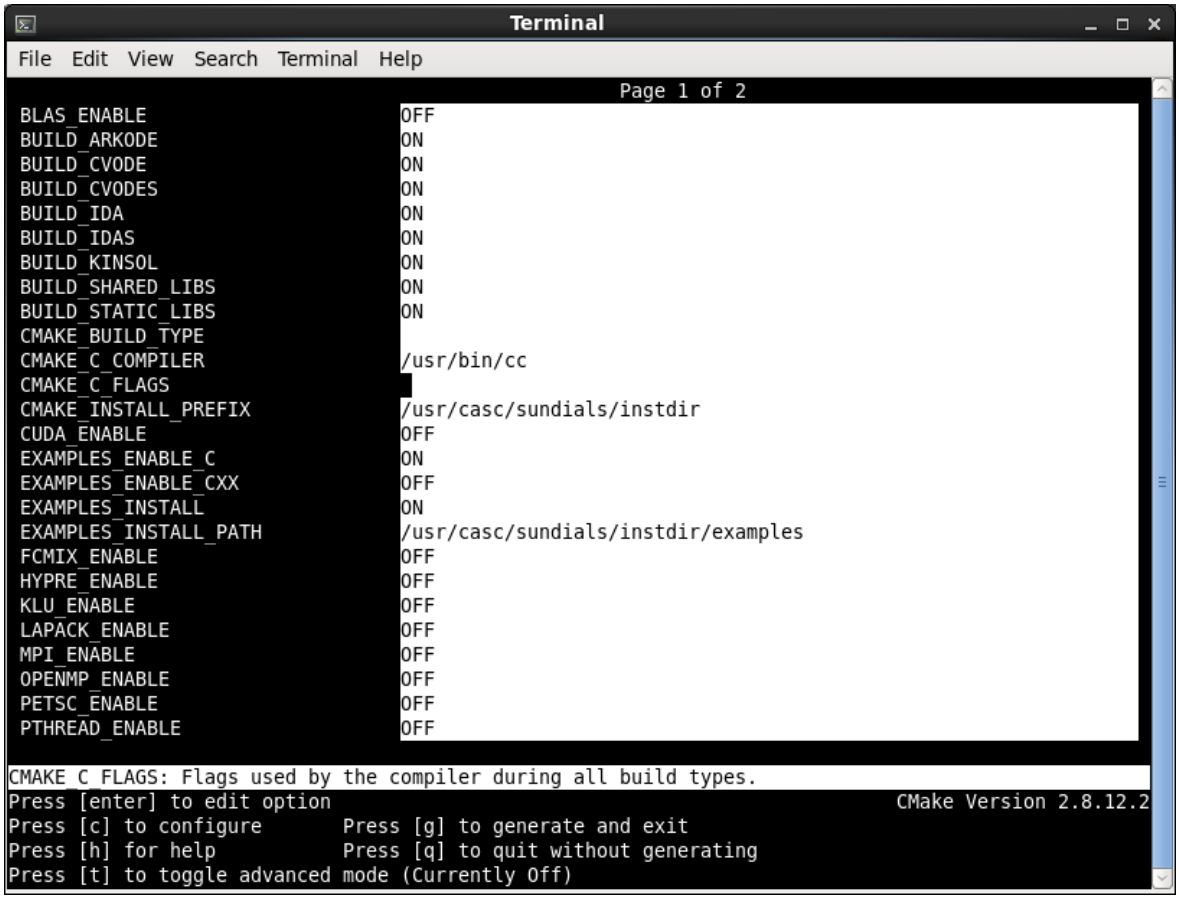

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the cmake command. The following will build the default configuration:

```
% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../srcdir
% make
% make install
```

A.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

`BLAS_ENABLE` - Enable BLAS support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with BLAS enabled in A.1.4.

`BLAS_LIBRARIES` - BLAS library
Default: /usr/lib/libblas.so

Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

BUILD_ARKODE - Build the ARKODE library
Default: ON

BUILD_CVODE - Build the CVODE library
Default: ON

BUILD_CVODES - Build the CVODES library
Default: ON

BUILD_IDA - Build the IDA library
Default: ON

BUILD_IDAS - Build the IDAS library
Default: ON

BUILD_KINSOL - Build the KINSOL library
Default: ON

BUILD_SHARED_LIBS - Build shared libraries
Default: ON

BUILD_STATIC_LIBS - Build static libraries
Default: ON

CMAKE_BUILD_TYPE - Choose the type of build, options are: None (CMAKE_C_FLAGS used), Debug, Release, RelWithDebInfo, and MinSizeRel
Default:
Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by CMAKE_<language>_FLAGS.

CMAKE_C_COMPILER - C compiler
Default: /usr/bin/cc

CMAKE_C_FLAGS - Flags for C compiler
Default:

CMAKE_C_FLAGS_DEBUG - Flags used by the C compiler during debug builds
Default: -g

CMAKE_C_FLAGS_MINSIZEREL - Flags used by the C compiler during release minsize builds
Default: -Os -DNDEBUG

CMAKE_C_FLAGS_RELEASE - Flags used by the C compiler during release builds
Default: -O3 -DNDEBUG

CMAKE_CXX_COMPILER - C++ compiler
Default: /usr/bin/c++
Note: A C++ compiler (and all related options) are only triggered if C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ applications by default without setting any additional configuration options.

CMAKE_CXX_FLAGS - Flags for C++ compiler
Default:

CMAKE_CXX_FLAGS_DEBUG - Flags used by the C++ compiler during debug builds
Default: -g

CMAKE_CXX_FLAGS_MINSIZEREL - Flags used by the C++ compiler during release minsize builds
Default: -Os -DNDEBUG

CMAKE_CXX_FLAGS_RELEASE - Flags used by the C++ compiler during release builds
Default: -O3 -DNDEBUG

CMAKE_Fortran_COMPILER - Fortran compiler
Default: /usr/bin/gfortran
Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (FCMIX_ENABLE is ON) or BLAS/LAPACK support is enabled (BLAS_ENABLE or LAPACK_ENABLE is ON).

CMAKE_Fortran_FLAGS - Flags for Fortran compiler
Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the Fortran compiler during debug builds
Default: -g

CMAKE_Fortran_FLAGS_MINSIZEREL - Flags used by the Fortran compiler during release minsize builds
Default: -Os

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the Fortran compiler during release builds
Default: -O3

CMAKE_INSTALL_PREFIX - Install path prefix, prepended onto install directories
Default: /usr/local
Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories include and lib of CMAKE_INSTALL_PREFIX, respectively.

CUDA_ENABLE - Build the SUNDIALS CUDA vector module.
Default: OFF

EXAMPLES_ENABLE_C - Build the SUNDIALS C examples
Default: ON

EXAMPLES_ENABLE_CUDA - Build the SUNDIALS CUDA examples
Default: OFF
Note: You need to enable CUDA support to build these examples.

EXAMPLES_ENABLE_CXX - Build the SUNDIALS C++ examples
Default: OFF

EXAMPLES_ENABLE_RAJA - Build the SUNDIALS RAJA examples
Default: OFF
Note: You need to enable CUDA and RAJA support to build these examples.

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples
Default: ON (if FCMIX_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90 examples
Default: OFF

EXAMPLES_INSTALL - Install example files
Default: ON
Note: This option is triggered when any of the SUNDIALS example programs are enabled (EXAMPLES_ENABLE_<language> is ON). If the user requires installation of example programs then the sources and sample output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by EXAMPLES_INSTALL_PATH. A CMake configuration

script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by `EXAMPLES_INSTALL_PATH`.

`EXAMPLES_INSTALL_PATH` - Output directory for installing example files
Default: /usr/local/examples
Note: The actual default value for this option will be an `examples` subdirectory created under `CMAKE_INSTALL_PREFIX`.

`FCMIX_ENABLE` - Enable Fortran-C support
Default: OFF

`HYPRE_ENABLE` - Enable *hypre* support
Default: OFF
Note: See additional information on building with *hypre* enabled in A.1.4.

`HYPRE_INCLUDE_DIR` - Path to *hypre* header files

`HYPRE_LIBRARY_DIR` - Path to *hypre* installed library files

`KLU_ENABLE` - Enable KLU support
Default: OFF
Note: See additional information on building with KLU enabled in A.1.4.

`KLU_INCLUDE_DIR` - Path to SuiteSparse header files

`KLU_LIBRARY_DIR` - Path to SuiteSparse installed library files

`LAPACK_ENABLE` - Enable LAPACK support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in A.1.4.

`LAPACK_LIBRARIES` - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
Note: CMake will search for libraries in your `LD_LIBRARY_PATH` prior to searching default system paths.

`MPI_ENABLE` - Enable MPI support (build the parallel nvector).
Default: OFF
Note: Setting this option to ON will trigger several additional options related to MPI.

`MPI_MPICC` - `mpicc` program
Default:

`MPI_MPICXX` - `mpicxx` program
Default:
Note: This option is triggered only if MPI is enabled (`MPI_ENABLE` is ON) and C++ examples are enabled (`EXAMPLES_ENABLE_CXX` is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than `MPI_ENABLE`.

`MPI_MPIF77` - `mpif77` program
Default:
Note: This option is triggered only if MPI is enabled (`MPI_ENABLE` is ON) and Fortran-C support is enabled (`FCMIX_ENABLE` is ON).

MPI_MPIF90 - mpif90 program
Default:
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON), Fortran-C support is enabled (FCMIX_ENABLE is ON), and Fortran90 examples are enabled (EXAMPLES_ENABLE_F90 is ON).

MPI_RUN_COMMAND - Specify run command for MPI
Default: mpirun Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON).

OPENMP_ENABLE - Enable OpenMP support (build the OpenMP nvector).
Default: OFF

PETSC_ENABLE - Enable PETSc support
Default: OFF
Note: See additional information on building with PETSc enabled in A.1.4.

PETSC_INCLUDE_DIR - Path to PETSc header files

PETSC_LIBRARY_DIR - Path to PETSc installed library files

PTHREAD_ENABLE - Enable Pthreads support (build the Pthreads nvector).
Default: OFF

RAJA_ENABLE - Enable RAJA support (build the RAJA nvector).
Default: OFF
Note: You need to enable CUDA in order to build the RAJA vector module.

SUNDIALS_INDEX_TYPE - Integer type used for SUNDIALS indices, options are: int32_t or int64_t
Default: int64_t

SUNDIALS_PRECISION - Precision used in SUNDIALS, options are: double, single, or extended
Default: double

SUPERLUMT_ENABLE - Enable SuperLU_MT support
Default: OFF
Note: See additional information on building with SuperLU_MT enabled in A.1.4.

SUPERLUMT_INCLUDE_DIR - Path to SuperLU_MT header files (typically SRC directory)

SUPERLUMT_LIBRARY_DIR - Path to SuperLU_MT installed library files

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP
Default: Pthread

USE_GENERIC_MATH - Use generic (stdc) math libraries
Default: ON

xSDK Configuration Options

SUNDIALS supports CMake configuration options defined by the Extreme-scale Scientific Software Development Kit (xSDK) community policies (see https://xsdk.info for more information). xSDK CMake options are unused by default but may be activated by setting USE_XSDK_DEFAULTS to ON.

When xSDK options are active, they will overwrite the corresponding SUNDIALS option and may have different default values (see details below). As such the equivalent SUNDIALS options should not be used when configuring with xSDK options. In the GUI front end to CMake (ccmake), setting USE_XSDK_DEFAULTS to ON will hide the corresponding SUNDIALS options as advanced CMake variables. During configuration, messages are output detailing which xSDK flags are active and the equivalent SUNDIALS options that are replaced. Below is a complete list xSDK options and the corresponding SUNDIALS options if applicable.

TPL_BLAS_LIBRARIES - BLAS library
Default: /usr/lib/libblas.so
SUNDIALS equivalent: BLAS_LIBRARIES
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

TPL_ENABLE_BLAS - Enable BLAS support
Default: OFF
SUNDIALS equivalent: BLAS_ENABLE

TPL_ENABLE_HYPRE - Enable *hypre* support
Default: OFF
SUNDIALS equivalent: HYPRE_ENABLE

TPL_ENABLE_KLU - Enable KLU support
Default: OFF
SUNDIALS equivalent: KLU_ENABLE

TPL_ENABLE_PETSC - Enable PETSc support
Default: OFF
SUNDIALS equivalent: PETSC_ENABLE

TPL_ENABLE_LAPACK - Enable LAPACK support
Default: OFF
SUNDIALS equivalent: LAPACK_ENABLE

TPL_ENABLE_SUPERLUMT - Enable SuperLU_MT support
Default: OFF
SUNDIALS equivalent: SUPERLUMT_ENABLE

TPL_HYPRE_INCLUDE_DIRS - Path to *hypre* header files
SUNDIALS equivalent: HYPRE_INCLUDE_DIR

TPL_HYPRE_LIBRARIES - *hypre* library
SUNDIALS equivalent: N/A

TPL_KLU_INCLUDE_DIRS - Path to KLU header files
SUNDIALS equivalent: KLU_INCLUDE_DIR

TPL_KLU_LIBRARIES - KLU library
SUNDIALS equivalent: N/A

TPL_LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
SUNDIALS equivalent: LAPACK_LIBRARIES
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

TPL_PETSC_INCLUDE_DIRS - Path to PETSc header files
SUNDIALS equivalent: PETSC_INCLUDE_DIR

TPL_PETSC_LIBRARIES - PETSc library
SUNDIALS equivalent: N/A

TPL_SUPERLUMT_INCLUDE_DIRS - Path to SuperLU_MT header files
SUNDIALS equivalent: SUPERLUMT_INCLUDE_DIR

TPL_SUPERLUMT_LIBRARIES - SuperLU_MT library
SUNDIALS equivalent: N/A

TPL_SUPERLUMT_THREAD_TYPE - SuperLU_MT library thread type
SUNDIALS equivalent: SUPERLUMT_THREAD_TYPE

USE_XSDK_DEFAULTS - Enable xSDK default configuration settings
Default: OFF
SUNDIALS equivalent: N/A
Note: Enabling xSDK defaults also sets CMAKE_BUILD_TYPE to Debug

XSDK_ENABLE_FORTRAN - Enable SUNDIALS Fortran interface
Default: OFF
SUNDIALS equivalent: FCMIX_ENABLE

XSDK_INDEX_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 32
SUNDIALS equivalent: SUNDIALS_INDEX_TYPE

XSDK_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad
Default: double
SUNDIALS equivalent: SUNDIALS_PRECISION

A.1.3 Configuration examples

The following examples will help demonstrate usage of the CMake configure options.
To configure SUNDIALS using the default C and Fortran compilers, and default mpicc and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> /home/myname/sundials/srcdir
%
% make install
%
```

To disable installation of the examples, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/srcdir
%
% make install
%
```

A.1.4 Working with external Libraries

The SUNDIALS suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries.

Building with BLAS

SUNDIALS does not utilize BLAS directly but it may be needed by other external libraries that SUNDIALS can be build with (e.g. LAPACK, PETSc, SuperLU_MT, etc.). To enable BLAS, set the BLAS_ENABLE option to ON. If the directory containing the BLAS library is in the LD_LIBRARY_PATH environment variable, CMake will set the BLAS_LIBRARIES variable accordingly, otherwise CMake will attempt to find the BLAS library in standard system locations. To explicitly tell CMake what libraries to use, the BLAS_LIBRARIES variable can be set to the desired library. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/myblaspath/lib/libblas.so \
> -DSUPERLUMT_ENABLE=ON \
> -DSUPERLUMT_INCLUDE_DIR=/mysuperlumtpath/SRC
> -DSUPERLUMT_LIBRARY_DIR=/mysuperlumtpath/lib
> /home/myname/sundials/srcdir
%
% make install
%
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.

Building with LAPACK

To enable LAPACK, set the LAPACK_ENABLE option to ON. If the directory containing the LAPACK library is in the LD_LIBRARY_PATH environment variable, CMake will set the LAPACK_LIBRARIES variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the LAPACK_LIBRARIES variable can be set to the desired libraries. When setting the LAPACK location explicitly the location of the corresponding BLAS library will also need to be set. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/mylapackpath/lib/libblas.so \
> -DLAPACK_ENABLE=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/srcdir
%
% make install
%
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.

Building with KLU

The KLU libraries are part of SuiteSparse, a suite of sparse matrix software, available from the Texas A&M University website: http://faculty.cse.tamu.edu/davis/suitesparse.html. SUNDIALS has been tested with SuiteSparse version 4.5.3. To enable KLU, set KLU_ENABLE to ON, set KLU_INCLUDE_DIR to the include path of the KLU installation and set KLU_LIBRARY_DIR to the lib path of the KLU

installation. The CMake configure will result in populating the following variables: AMD_LIBRARY, AMD_LIBRARY_DIR, BTF_LIBRARY, BTF_LIBRARY_DIR, COLAMD_LIBRARY, COLAMD_LIBRARY_DIR, and KLU_LIBRARY.

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt. SUNDIALS has been tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set SUPERLUMT_ENABLE to ON, set SUPERLUMT_INCLUDE_DIR to the SRC path of the SuperLU_MT installation, and set the variable SUPERLUMT_LIBRARY_DIR to the lib path of the SuperLU_MT installation. At the same time, the variable SUPERLUMT_THREAD_TYPE must be set to either Pthread or OpenMP.

Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either OPENMP_ENABLE or PTHREAD_ENABLE set to ON then SuperLU_MT should be set to use the same threading type.

Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: http://www.mcs.anl.gov/petsc. SUNDIALS has been tested with PETSc version 3.7.2. To enable PETSc, set PETSC_ENABLE to ON, set PETSC_INCLUDE_DIR to the include path of the PETSc installation, and set the variable PETSC_LIBRARY_DIR to the lib path of the PETSc installation.

Building with *hypre*

The *hypre* libraries are available for download from the Lawrence Livermore National Laboratory website: http://computation.llnl.gov/projects/hypre. SUNDIALS has been tested with *hypre* version 2.11.1. To enable *hypre*, set HYPRE_ENABLE to ON, set HYPRE_INCLUDE_DIR to the include path of the *hypre* installation, and set the variable HYPRE_LIBRARY_DIR to the lib path of the *hypre* installation.

Building with CUDA

SUNDIALS CUDA modules and examples are tested with version 8.0 of the CUDA toolkit. To build them, you need to install the Toolkit and compatible NVIDIA drivers. Both are available for download from NVIDIA website: https://developer.nvidia.com/cuda-downloads. To enable CUDA, set CUDA_ENABLE to ON. If you installed CUDA in a nonstandard location, you may be prompted to set the variable CUDA_TOOLKIT_ROOT_DIR with your CUDA Toolkit installation path. To enable CUDA examples, set EXAMPLES_ENABLE_CUDA to ON.

Building with RAJA

To build SUNDIALS RAJA modules you need to enable SUNDIALS CUDA support, first. You also need a CUDA-enabled RAJA installation on your system. RAJA is free software, developed by Lawrence Livermore National Laboratory, and can be obtained from https://github.com/LLNL/RAJA. Next you need to set RAJA_ENABLE to ON, to enable building the RAJA vector module, and EXAMPLES_ENABLE_RAJA to ON to build the RAJA examples. If you installed RAJA to a nonstandard location you will be prompted to set the variable RAJA_DIR with the path to the RAJA CMake configuration file. SUNDIALS was tested with RAJA version 0.3.

A.2 Building and Running Examples

Each of the SUNDIALS solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set at least of the EXAMPLES_ENABLE_<language> options to ON, and set EXAMPLES_INSTALL to ON. Specify the installation path for the examples with the variable

EXAMPLES_INSTALL_PATH. CMake will generate CMakeLists.txt configuration files (and Makefile files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

Either the CMakeLists.txt file or the traditional Makefile may be used to build the examples as well as serve as a template for creating user developed solutions. To use the supplied Makefile simply run make to compile and generate the executables. To use CMake from within the installed example directory, run cmake (or ccmake to use the GUI) followed by make to compile the example code. Note that if CMake is used, it will overwrite the traditional Makefile with a new CMake-generated Makefile. The resulting output from running the examples can be compared with example output bundled in the SUNDIALS distribution.

NOTE: There will potentially be differences in the output due to machine architecture, compiler versions, use of third party libraries etc.

A.3 Configuring, building, and installing on Windows

CMake can also be used to build SUNDIALS on Windows. To build SUNDIALS for use with Visual Studio the following steps should be performed:

1. Unzip the downloaded tar file(s) into a directory. This will be the *srcdir*
2. Create a separate *builddir*
3. Open a Visual Studio Command Prompt and cd to *builddir*
4. Run cmake-gui ../*srcdir*
   (a) Hit Configure
   (b) Check/Uncheck solvers to be built
   (c) Change CMAKE_INSTALL_PREFIX to *instdir*
   (d) Set other options as desired
   (e) Hit Generate
5. Back in the VS Command Window:
   (a) Run msbuild ALL_BUILD.vcxproj
   (b) Run msbuild INSTALL.vcxproj

The resulting libraries will be in the *instdir*. The SUNDIALS project can also now be opened in Visual Studio. Double click on the ALL_BUILD.vcxproj file to open the project. Build the whole *solution* to create the SUNDIALS libraries. To use the SUNDIALS libraries in your own projects, you must set the include directories for your project, add the SUNDIALS libraries to your project solution, and set the SUNDIALS libraries as dependencies for your project.

A.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

```
% make install
```

will install the libraries under *libdir* and the public header files under *includedir*. The values for these directories are *instdir*/lib and *instdir*/include, respectively. The location can be changed by setting the CMake variable CMAKE_INSTALL_PREFIX. Although all installed libraries reside under *libdir*/lib, the public header files are further organized into subdirectories under *includedir*/include.

The installed libraries and exported header files are listed for reference in Tables A.1 and A.2. The file extension *.lib* is typically .so for shared libraries and .a for static libraries. Note that, in the Tables, names are relative to *libdir* for libraries and to *includedir* for header files.

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the *includedir*/include/sundials directory since they are explicitly included by the appropriate solver header files (*e.g.*, cvode_dense.h includes sundials_dense.h). However, it is both legal and safe to do so, and would be useful, for example, if the functions declared in sundials_dense.h are to be used in building a preconditioner.

Table A.1: SUNDIALS libraries and header files

SHARED	Libraries	n/a	
	Header files	sundials/sundials_config.h	sundials/sundials_fconfig.h
		sundials/sundials_types.h	sundials/sundials_math.h
		sundials/sundials_nvector.h	sundials/sundials_fnvector.h
		sundials/sundials_iterative.h	sundials/sundials_direct.h
		sundials/sundials_dense.h	sundials/sundials_band.h
		sundials/sundials_matrix.h	sundials/sundials_linearsolver.h
		sundials/sundials_version.h	
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib*	libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h	
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib*	libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h	
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.*lib*	libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h	
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.*lib*	libsundials_fnvecpthreads.a
	Header files	nvector/nvector_pthreads.h	
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.*lib*	
		libsundials_fsunmatrixband.a	
	Header files	sunmatrix/sunmatrix_band.h	
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.*lib*	
		libsundials_fsunmatrixdense.a	
	Header files	sunmatrix/sunmatrix_dense.h	
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse.*lib*	
		libsundials_fsunmatrixsparse.a	
	Header files	sunmatrix/sunmatrix_sparse.h	
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.*lib*	
		libsundials_fsunlinsolband.a	
	Header files	sunlinsol/sunlinsol_band.h	
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.*lib*	
		libsundials_fsunlinsoldense.a	
	Header files	sunlinsol/sunlinsol_dense.h	
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.*lib*	
		libsundials_fsunlinsolklu.a	
	Header files	sunlinsol/sunlinsol_klu.h	
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.*lib*	
		libsundials_fsunlinsollapackband.a	
	Header files	sunlinsol/sunlinsol_lapackband.h	
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.*lib*	
		libsundials_fsunlinsollapackdense.a	
	Header files	sunlinsol/sunlinsol_lapackdense.h	
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.*lib*	
		libsundials_fsunlinsolpcg.a	
	Header files	sunlinsol/sunlinsol_pcg.h	
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.*lib*	
		libsundials_fsunlinsolspbcgs.a	
	Header files	sunlinsol/sunlinsol_spbcgs.h	

Table A.2: SUNDIALS libraries and header files (cont.)

SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.*lib* libsundials_fsunlinsolspfgmr.a	
	Header files	sunlinsol/sunlinsol_spfgmr.h	
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.*lib* libsundials_fsunlinsolspgmr.a	
	Header files	sunlinsol/sunlinsol_spgmr.h	
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.*lib* libsundials_fsunlinsolsptfqmr.a	
	Header files	sunlinsol/sunlinsol_sptfqmr.h	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.*lib* libsundials_fsunlinsolsuperlumt.a	
	Header files	sunlinsol/sunlinsol_superlumt.h	
CVODE	Libraries	libsundials_cvode.*lib*	libsundials_fcvode.a
	Header files	cvode/cvode.h cvode/cvode_direct.h cvode/cvode_bandpre.h	cvode/cvode_impl.h cvode/cvode_spils.h cvode/cvode_bbdpre.h
CVODES	Libraries	libsundials_cvodes.*lib*	
	Header files	cvodes/cvodes.h cvodes/cvodes_direct.h cvodes/cvodes_bandpre.h	cvodes/cvodes_impl.h cvodes/cvodes_spils.h cvodes/cvodes_bbdpre.h
ARKODE	Libraries	libsundials_arkode.*lib*	libsundials_farkode.a
	Header files	arkode/arkode.h arkode/arkode_direct.h arkode/arkode_bandpre.h	arkode/arkode_impl.h arkode/arkode_spils.h arkode/arkode_bbdpre.h
IDA	Libraries	libsundials_ida.*lib*	libsundials_fida.a
	Header files	ida/ida.h ida/ida_direct.h ida/ida_bbdpre.h	ida/ida_impl.h ida/ida_spils.h
IDAS	Libraries	libsundials_idas.*lib*	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_bbdpre.h	idas/idas_impl.h idas/idas_spils.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a
	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_bbdpre.h	kinsol/kinsol_impl.h kinsol/kinsol_spils.h

Appendix B

IDAS Constants

Below we list all input and output constants used by the main solver and linear solver modules, together with their numerical values and a short description of their meaning.

B.1 IDAS input constants

IDAS **main solver module**		
IDA_NORMAL	1	Solver returns at specified output time.
IDA_ONE_STEP	2	Solver returns after each successful step.
IDA_SIMULTANEOUS	1	Simultaneous corrector forward sensitivity method.
IDA_STAGGERED	2	Staggered corrector forward sensitivity method.
IDA_CENTERED	1	Central difference quotient approximation (2^{nd} order) of the sensitivity RHS.
IDA_FORWARD	2	Forward difference quotient approximation (1^{st} order) of the sensitivity RHS.
IDA_YA_YDP_INIT	1	Compute y_a and $\dot{y}_d$, given y_d.
IDA_Y_INIT	2	Compute y, given $\dot{y}$.

IDAS **adjoint solver module**		
IDA_HERMITE	1	Use Hermite interpolation.
IDA_POLYNOMIAL	2	Use variable-degree polynomial interpolation.

Iterative linear solver module		
PREC_NONE	0	No preconditioning
PREC_LEFT	1	Preconditioning on the left.
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

B.2 IDAS output constants

IDAS **main solver module**

IDA_SUCCESS	0	Successful function return.
IDA_TSTOP_RETURN	1	IDASolve succeeded by reaching the specified stopping point.
IDA_ROOT_RETURN	2	IDASolve succeeded and found one or more roots.
IDA_WARNING	99	IDASolve succeeded but an unusual situation occurred.
IDA_TOO_MUCH_WORK	-1	The solver took mxstep internal steps but could not reach tout.
IDA_TOO_MUCH_ACC	-2	The solver could not satisfy the accuracy demanded by the user for some internal step.
IDA_ERR_FAIL	-3	Error test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_CONV_FAIL	-4	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_LINIT_FAIL	-5	The linear solver's initialization function failed.
IDA_LSETUP_FAIL	-6	The linear solver's setup function failed in an unrecoverable manner.
IDA_LSOLVE_FAIL	-7	The linear solver's solve function failed in an unrecoverable manner.
IDA_RES_FAIL	-8	The user-provided residual function failed in an unrecoverable manner.
IDA_REP_RES_FAIL	-9	The user-provided residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_RTFUNC_FAIL	-10	The rootfinding function failed in an unrecoverable manner.
IDA_CONSTR_FAIL	-11	The inequality constraints were violated and the solver was unable to recover.
IDA_FIRST_RES_FAIL	-12	The user-provided residual function failed recoverably on the first call.
IDA_LINESEARCH_FAIL	-13	The line search failed.
IDA_NO_RECOVERY	-14	The residual function, linear solver setup function, or linear solver solve function had a recoverable failure, but IDACalcIC could not recover.
IDA_MEM_NULL	-20	The ida_mem argument was NULL.
IDA_MEM_FAIL	-21	A memory allocation failed.
IDA_ILL_INPUT	-22	One of the function inputs is illegal.
IDA_NO_MALLOC	-23	The IDAS memory was not allocated by a call to IDAInit.
IDA_BAD_EWT	-24	Zero value of some error weight component.
IDA_BAD_K	-25	The k-th derivative is not available.
IDA_BAD_T	-26	The time t is outside the last step taken.
IDA_BAD_DKY	-27	The vector argument where derivative should be stored is NULL.
IDA_NO_QUAD	-30	Quadratures were not initialized.
IDA_QRHS_FAIL	-31	The user-provided right-hand side function for quadratures failed in an unrecoverable manner.
IDA_FIRST_QRHS_ERR	-32	The user-provided right-hand side function for quadratures failed in an unrecoverable manner on the first call.
IDA_REP_QRHS_ERR	-33	The user-provided right-hand side repeatedly returned a recoverable error flag, but the solver was unable to recover.

IDA_NO_SENS	-40	Sensitivities were not initialized.
IDA_SRES_FAIL	-41	The user-provided sensitivity residual function failed in an unrecoverable manner.
IDA_REP_SRES_ERR	-42	The user-provided sensitivity residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_BAD_IS	-43	The sensitivity identifier is not valid.
IDA_NO_QUADSENS	-50	Sensitivity-dependent quadratures were not initialized.
IDA_QSRHS_FAIL	-51	The user-provided sensitivity-dependent quadrature right-hand side function failed in an unrecoverable manner.
IDA_FIRST_QSRHS_ERR	-52	The user-provided sensitivity-dependent quadrature right-hand side function failed in an unrecoverable manner on the first call.
IDA_REP_QSRHS_ERR	-53	The user-provided sensitivity-dependent quadrature right-hand side repeatedly returned a recoverable error flag, but the solver was unable to recover.

IDAS **adjoint solver module**

IDA_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDA_NO_FWD	-102	IDASolveF has not been previously called.
IDA_NO_BCK	-103	No backward problem was specified.
IDA_BAD_TBO	-104	The desired output for backward problem is outside the interval over which the forward problem was solved.
IDA_REIFWD_FAIL	-105	No checkpoint is available for this hot start.
IDA_FWD_FAIL	-106	IDASolveB failed because IDASolve was unable to store data between two consecutive checkpoints.
IDA_GETY_BADT	-107	Wrong time in interpolation function.

IDADLS **linear solver modules**

IDADLS_SUCCESS	0	Successful function return.
IDADLS_MEM_NULL	-1	The ida_mem argument was NULL.
IDADLS_LMEM_NULL	-2	The IDADLS linear solver has not been initialized.
IDADLS_ILL_INPUT	-3	The IDADLS solver is not compatible with the current NVECTOR module.
IDADLS_MEM_FAIL	-4	A memory allocation request failed.
IDADLS_JACFUNC_UNRECVR	-5	The Jacobian function failed in an unrecoverable manner.
IDADLS_JACFUNC_RECVR	-6	The Jacobian function had a recoverable error.
IDADLS_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDADLS_LMEMB_NULL	-102	The linear solver was not initialized for the backward phase.

IDASLS **linear solver module**

IDASLS_SUCCESS	0	Successful function return.
IDASLS_MEM_NULL	-1	The ida_mem argument was NULL.
IDASLS_LMEM_NULL	-2	The IDASLS linear solver has not been initialized.
IDASLS_ILL_INPUT	-3	The IDASLS solver is not compatible with the current NVECTOR module or other input is invalid.
IDASLS_MEM_FAIL	-4	A memory allocation request failed.
IDASLS_JAC_NOSET	-5	The Jacobian evaluation routine was not been set before the linear solver setup routine was called.
IDASLS_PACKAGE_FAIL	-6	An external package call return a failure error code.
IDASLS_JACFUNC_UNRECVR	-7	The Jacobian function failed in an unrecoverable manner.
IDASLS_JACFUNC_RECVR	-8	The Jacobian function had a recoverable error.
IDASLS_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDASLS_LMEMB_NULL	-102	The linear solver was not initialized for the backward phase.

IDASPILS **linear solver modules**

IDASPILS_SUCCESS	0	Successful function return.
IDASPILS_MEM_NULL	-1	The ida_mem argument was NULL.
IDASPILS_LMEM_NULL	-2	The IDASPILS linear solver has not been initialized.
IDASPILS_ILL_INPUT	-3	The IDASPILS solver is not compatible with the current NVECTOR module.
IDASPILS_MEM_FAIL	-4	A memory allocation request failed.
IDASPILS_PMEM_NULL	-5	The preconditioner module has not been initialized.
IDASPILS_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDASPILS_LMEMB_NULL	-102	The linear solver was not initialized for the backward phase.

SPGMR **generic linear solver module**

SPGMR_SUCCESS	0	Converged.
SPGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPGMR_CONV_FAIL	2	Failure to converge.
SPGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPGMR_ATIMES_FAIL_REC	5	The Jacobian-times-vector function failed recoverably.
SPGMR_PSET_FAIL_REC	6	The preconditioner setup routine failed recoverably.
SPGMR_MEM_NULL	-1	The SPGMR memory is NULL
SPGMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPGMR_QRSOL_FAIL	-5	The matrix R was found to be singular during the QR solve phase.

SPGMR_PSET_FAIL_UNREC	-6	The preconditioner setup routine failed unrecoverably.

SPFGMR generic linear solver module (only available in KINSOL and ARKODE)

SPFGMR_SUCCESS	0	Converged.
SPFGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPFGMR_CONV_FAIL	2	Failure to converge.
SPFGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPFGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPFGMR_ATIMES_FAIL_REC	5	The Jacobian-times-vector function failed recoverably.
SPFGMR_PSET_FAIL_REC	6	The preconditioner setup routine failed recoverably.
SPFGMR_MEM_NULL	-1	The SPFGMR memory is NULL
SPFGMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPFGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPFGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPFGMR_QRSOL_FAIL	-5	The matrix R was found to be singular during the QR solve phase.
SPFGMR_PSET_FAIL_UNREC	-6	The preconditioner setup routine failed unrecoverably.

SPBCGS generic linear solver module

SPBCG_SUCCESS	0	Converged.
SPBCG_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPBCG_CONV_FAIL	2	Failure to converge.
SPBCG_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPBCG_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPBCG_PSET_FAIL_REC	5	The preconditioner setup routine failed recoverably.
SPBCG_MEM_NULL	-1	The SPBCGS memory is NULL
SPBCG_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPBCG_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPBCG_PSET_FAIL_UNREC	-4	The preconditioner setup routine failed unrecoverably.

SPTFQMR generic linear solver module

SPTFQMR_SUCCESS	0	Converged.
SPTFQMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPTFQMR_CONV_FAIL	2	Failure to converge.
SPTFQMR_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPTFQMR_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPTFQMR_PSET_FAIL_REC	5	The preconditioner setup routine failed recoverably.
SPTFQMR_MEM_NULL	-1	The SPTFQMR memory is NULL
SPTFQMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed.
SPTFQMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPTFQMR_PSET_FAIL_UNREC	-4	The preconditioner setup routine failed unrecoverably.

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