User Documentation for IDAS v3.0.0 (SUNDIALS v4.0.0)

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Chapter 1

Introduction

IDAS is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [26]. 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 [7, 8]; 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 and matrices 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 [27, 15] and PVODE [11, 12], the DAE solver IDA [30] on which IDAS is based, the sensitivity-enabled ODE solver CVODES [28, 42], and also the nonlinear system solver KINSOL [16].

At present, IDAS may utilize a variety of Krylov methods provided in SUNDIALS that can be used in conjuction with Newton iteration: these include the GMRES (Generalized Minimal RESidual) [41], FGMRES (Flexible Generalized Minimum RESidual) [40], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [44], TFQMR (Transpose-Free Quasi-Minimal Residual) [23], and PCG (Preconditioned Conjugate Gradient) [24] linear iterative methods. As Krylov methods, these require little 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 Krylov methods in SUNDIALS, we recommend GMRES as the best overall choice. However, users are encouraged to compare all options, 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. FGMRES has an advantage in that it is designed to support preconditioners that vary between iterations (e.g. iterative methods). PCG exhibits rapid convergence and minimal workspace vectors, but only works for symmetric linear systems.

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 v3.0.0

IDAS' previous direct and iterative linear solver interfaces, IDADLS and IDASPILS, have been merged into a single unified linear solver interface, IDALS, to support any valid SUNLINSOL module. This includes the "DIRECT" and "ITERATIVE" types as well as the new "MATRIX_ITERATIVE" type. Details regarding how IDALS utilizes linear solvers of each type as well as discussion regarding intended use cases for user-supplied SUNLINSOL implementations are included in Chapter 9. All IDAS example programs and the standalone linear solver examples have been updated to use the unified linear solver interface.

The unified interface for the new IDALS module is very similar to the previous IDADLS and IDASPILS interfaces. To minimize challenges in user migration to the new names, the previous C routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon.

The names of all constructor routines for SUNDIALS-provided SUNLINSOL implementations have been updated to follow the naming convention `SUNLinSol_*` where `*` is the name of the linear solver. The new names are `SUNLinSol_Band`, `SUNLinSol_Dense`, `SUNLinSol_KLU`, `SUNLinSol_LapackBand`, `SUNLinSol_LapackDense`, `SUNLinSol_PCG`, `SUNLinSol_SPBCGS`, `SUNLinSol_SPFGMR`, `SUNLinSol_SPGMR`, `SUNLinSol_SPTFQMR`, and `SUNLinSol_SuperLUMT`. Solver-specific "set" routine names have been similarly standardized. To minimize challenges in user migration to the new names, the previous routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon. All IDAS example programs and the standalone linear solver examples have been updated to use the new naming convention.

The `SUNBandMatrix` constructor has been simplified to remove the storage upper bandwidth argument.

SUNDIALS integrators have been updated to utilize generic nonlinear solver modules defined through the SUNNONLINSOL API. This API will ease the addition of new nonlinear solver options and allow for external or user-supplied nonlinear solvers. The SUNNONLINSOL API and SUNDIALS provided modules are described in Chapter 10 and follow the same object oriented design and implementation used by the NVECTOR, SUNMATRIX, and SUNLINSOL modules. Currently two SUNNONLINSOL implementations are provided, SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT. These replicate the previous integrator specific implementations of a Newton iteration and a fixed-point iteration (previously referred to as a functional iteration), respectively. Note the SUNNONLINSOL_FIXEDPOINT module can optionally utilize Anderson's method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all IDAS example programs have been updated to use generic SUNNONLINSOL modules.

By default IDAS uses the SUNNONLINSOL_NEWTON module. Since IDAS previously only used an internal implementation of a Newton iteration no changes are required to user programs and functions for setting the nonlinear solver options (e.g., `IDASetMaxNonlinIters`) or getting nonlinear solver statistics (e.g., `IDAGetNumNonlinSolvIters`) remain unchanged and internally call generic SUNNONLINSOL functions as needed. While SUNDIALS includes a fixed-point nonlinear solver module, it is not currently supported in IDAS. For details on attaching a user-supplied nonlinear solver to IDAS see Chapter 4, 5, and 6.

Three fused vector operations and seven vector array operations have been added to the NVECTOR API. These *optional* operations are disabled by default and may be activated by calling vector specific routines after creating an NVECTOR (see Chapter 7 for more details). The new operations are `N_VLinearCombination`, `N_VScaleAddMulti`, and `N_VDotProdMulti` and the vector array operations are `N_VLinearCombinationVectorArray`, `N_VScaleVectorArray`, `N_VConstVectorArray`, `N_VWrmsNormVectorArray`, `N_VWrmsNormMaskVectorArray`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. If an NVECTOR implementation defines any of these operations as `NULL`, then standard NVECTOR operations will automatically be called as necessary to complete the computation.

Multiple updates to NVECTOR_CUDA were made:

- Changed `N_VGetLength_Cuda` to return the global vector length instead of the local vector length.
- Added `N_VGetLocalLength_Cuda` to return the local vector length.
- Added `N_VGetMPIComm_Cuda` to return the MPI communicator used.
- Removed the accessor functions in the namespace suncudavec.
- Changed the `N_VMake_Cuda` function to take a host data pointer and a device data pointer instead of an `N_VectorContent_Cuda` object.
- Added the ability to set the `cudaStream_t` used for execution of the NVECTOR_CUDA kernels. See the function `N_VSetCudaStreams_Cuda`.
- Added `N_VNewManaged_Cuda`, `N_VMakeManaged_Cuda`, and `N_VIsManagedMemory_Cuda` functions to accommodate using managed memory with the NVECTOR_CUDA.

Multiple changes to NVECTOR_RAJA were made:

- Changed `N_VGetLength_Raja` to return the global vector length instead of the local vector length.
- Added `N_VGetLocalLength_Raja` to return the local vector length.
- Added `N_VGetMPIComm_Raja` to return the MPI communicator used.
- Removed the accessor functions in the namespace suncudavec.

A new NVECTOR implementation for leveraging OpenMP 4.5+ device offloading has been added, NVECTOR_OPENMPDEV. See §7.10 for more details.

Changes in v2.2.1

The changes in this minor release include the following:

- Fixed a bug in the CUDA NVECTOR where the `N_VInvTest` operation could write beyond the allocated vector data.
- Fixed library installation path for multiarch systems. This fix changes the default library installation path to `CMAKE_INSTALL_PREFIX/CMAKE_INSTALL_LIBDIR` from `CMAKE_INSTALL_PREFIX/lib`. `CMAKE_INSTALL_LIBDIR` is automatically set, but is available as a CMake option that can modified.

Changes in v2.2.0

Fixed a bug in IDAS where the saved residual value used in the nonlinear solve for consistent initial conditions was passed as temporary workspace and could be overwritten.

Fixed a thread-safety issue when using ajdoint sensitivity analysis.

Fixed a problem with setting `sunindextype` which would occur with some compilers (e.g. armclang) that did not define `__STDC_VERSION__`.

Added hybrid MPI/CUDA and MPI/RAJA vectors to allow use of more than one MPI rank when using a GPU system. The vectors assume one GPU device per MPI rank.

Changed the name of the RAJA NVECTOR library to `libsundials_nveccudaraja.lib` from `libsundials_nvecraja.lib` to better reflect that we only support CUDA as a backend for RAJA currently.

Several changes were made to the build system:

- CMake 3.1.3 is now the minimum required CMake version.
- Deprecate the behavior of the `SUNDIALS_INDEX_TYPE` CMake option and added the `SUNDIALS_INDEX_SIZE` CMake option to select the `sunindextype` integer size.
- The native CMake FindMPI module is now used to locate an MPI installation.
- If MPI is enabled and MPI compiler wrappers are not set, the build system will check if `CMAKE_<language>_COMPILER` can compile MPI programs before trying to locate and use an MPI installation.
- The previous options for setting MPI compiler wrappers and the executable for running MPI programs have been have been depreated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPI_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.
- When a Fortran name-mangling scheme is needed (e.g., `LAPACK_ENABLE` is `ON`) the build system will infer the scheme from the Fortran compiler. If a Fortran compiler is not available or the inferred or default scheme needs to be overridden, the advanced options `SUNDIALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` can be used to manually set the name-mangling scheme and bypass trying to infer the scheme.
- Parts of the main CMakeLists.txt file were moved to new files in the `src` and `example` directories to make the CMake configuration file structure more modular.

Changes in v2.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using rpath by default to locate shared libraries on OSX.
- Fixed Windows specific problem where `sunindextype` was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows `sunindextype` is now defined as the MSVC basic type `__int64`.
- Added sparse SUNMatrix "Reallocate" routine to allow specification of the nonzero storage.

- Updated the KLU SUNLINSOL module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.
- Updated the "ScaleAdd" and "ScaleAddI" implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum $I + \gamma J$ manually (with zero entries if needed).
- Changed the LICENSE install path to `instdir/include/sundials`.

Changes in v2.1.1

The changes in this minor release include the following:

- Fixed a potential memory leak in the SPGMR and SPFGMR linear solvers: if "Initialize" was called multiple times then the solver memory was reallocated (without being freed).
- Updated KLU SUNLinearSolver module to use a `typedef` for the precision-specific solve function to be used (to avoid compiler warnings).
- Added missing typecasts for some `(void*)` pointers (again, to avoid compiler warnings).
- Bugfix in `sunmatrix_sparse.c` where we had used `int` instead of `sunindextype` in one location.
- Added missing `#include <stdio.h>` in NVECTOR and SUNMATRIX header files.
- Added missing prototype for `IDASpilsGetNumJTSetupEvals`.
- Fixed an indexing bug in the CUDA NVECTOR implementation of `N_VWrmsNormMask` and revised the RAJA NVECTOR implementation of `N_VWrmsNormMask` to work with mask arrays using values other than zero or one. Replaced `double` with `realtype` in the RAJA vector test functions.

In addition to the changes above, minor corrections were also made to the example programs, build system, and user documentation.

Changes in v2.1.0

Added NVECTOR print functions that write vector data to a specified file (e.g., `N_VPrintFile_Serial`).

Added `make test` and `make test_install` options to the build system for testing SUNDIALS after building with `make` and installing with `make install` respectively.

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 to 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: SUNDIALS native dense, SUNDIALS native banded, LAPACK dense, LAPACK band, KLU, SuperLU_MT, SPGMR, SPBCGS, SPTFQMR, SPFGMR, and 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 and files to utilize the 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` is defined to be `int32_t` or `int64_t` when portable types are supported, otherwise it is defined as `int` or `long int`. The Fortran interfaces continue to use `long int` for indices, except for their sparse matrix interface that now uses the new `sunindextype`. This new flexible capability for index types includes interfaces to PETSc, hypre, SuperLU_MT, and KLU with either 32-bit or 64-bit capabilities depending how the user configures SUNDIALS.

To avoid potential namespace conflicts, the macros defining `booleantype` values `TRUE` and `FALSE` have been changed to `SUNTRUE` and `SUNFALSE` respectively.

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.

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.

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

In addition, numerous changes were made to the build system. These include the addition of separate `BLAS_ENABLE` and `BLAS_LIBRARIES` 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 `EXAMPLES_ENABLE` to `EXAMPLES_ENABLE_C`, changing `CXX_ENABLE` to `EXAMPLES_ENABLE_CXX`, changing `F90_ENABLE` to `EXAMPLES_ENABLE_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 8 gives a brief overview of the generic SUNMATRIX module shared among the various components of SUNDIALS, and details on the SUNMATRIX implementations provided with SUNDIALS: a dense implementation (§8.2), a banded implementation (§8.3) and a sparse implementation (§8.4).
- Chapter 9 gives a brief overview of the generic SUNLINSOL module shared among the various components of SUNDIALS. This chapter contains details on the SUNLINSOL implementations provided with SUNDIALS. The chapter also contains details on the SUNLINSOL implementations provided with SUNDIALS that interface with external linear solver libraries.
- Chapter 10 describes the SUNNONLINSOL API and nonlinear solver implementations shared among the various components of SUNDIALS.
- 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).

Finally, 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 IDALS, 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 [8]. 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, IDA 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 [4]. 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:

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

By default IDAS solves (2.4) with a Newton iteration but IDAS also allows for user-defined nonlinear solvers (see Chapter 10). Each Newton iteration requires the soution of a linear system 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 iteration, IDAS provides several choices, including the option of a user-supplied linear solver module (see Chapter 9). The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices 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 [17, 1], or the thread-enabled SuperLU_MT sparse solver library [35, 19, 2] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of IDAS],
- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver without restarts,
- SPFGMR, a scaled preconditioned FGMRES (Flexible Generalized Minimal Residual method) solver,
- SPBCGS, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver,
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver, or
- PCG, a scaled preconditioned CG (Conjugate Gradient method) solver.

For large stiff systems, where direct methods are not feasible, the combination of a BDF integrator and a preconditioned Krylov method 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 [6]. For the *spils* linear solvers with IDAS, preconditioning is allowed only on the left (see §2.2). Note that the dense, band, and sparse direct linear solvers can only be used with serial and threaded vector representations.

In the process of controlling errors at various levels, IDAS uses a weighted root-mean-square norm, denoted $\|\cdot\|_{\text{WRMS}}$, 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

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

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 matrix-based linear solver, the default Newton iteration is a Modified Newton iteration, in that the Jacobian J is fixed (and usually out of date) throughout the nonlinear iterations, with a coefficient $\bar{\alpha}$ in place of α in J. However, in the case that a matrix-free iterative linear solver is used, the default Newton iteration is an Inexact Newton iteration, in which J is applied in a matrix-free manner, with matrix-vector products Jv obtained by either difference quotients or a user-supplied routine. In this case, the linear residual $J\Delta y + G$ is nonzero but controlled. With the default Newton iteration, the matrix J and preconditioner matrix P are updated as infrequently as possible to balance the high costs of matrix operations against other costs. Specifically, this matrix update occurs 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 default stopping test for nonlinear solver iterations 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 nonlinear solver 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 $\alpha \ne \bar{\alpha}$. Note that at $m = 1$, the convergence test (2.8) uses an old value for S. Therefore, at the first nonlinear solver 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 nonlinear 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 number of allowable nonlinear iterations and the maximum number of nonlinear convergence failures can be changed by the user from their default values.

When an iterative method 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 nonlinear iteration, i.e., $\|P^{-1}(Jx+G)\| < 0.05 \cdot 0.33$. The safety factor 0.05 can be changed by the user.

When the Jacobian is stored using either dense or band SUNMATRIX objects, 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

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

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). We note that with sparse and user-supplied SUNMATRIX objects, the Jacobian *must* be supplied by a user routine.

In the case of an iterative linear solver, 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 $\sigma = \sqrt{N}$. As an option, the user can specify a constant factor that is inserted into this expression for σ.

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 [4] 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 nonlinear 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 nonlinear solver that requires the solution of a linear system of the form $J\Delta y = -G$ (e.g., the default Newton iteration), IDAS makes repeated use of a linear solver. If this linear system solve is done with one of the scaled preconditioned iterative linear solvers supplied with SUNDIALS, 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 nonlinear 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 [6] for an extensive study of preconditioners for reaction-transport systems).

Typical preconditioners used with IDAS are based on approximations to the 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 nonlinear solver 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 [25]. 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 [14], 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 [34]. 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 [37], 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 [22], 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 [13].

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 [13].

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 [13] 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]

[1] The degree of the interpolation polynomial is always that of the current BDF order for the forward interpolation at

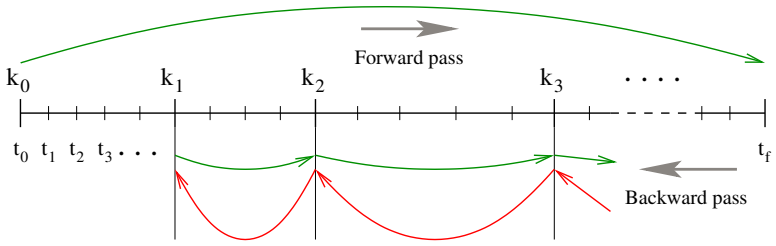


Figure 2.1: Illustration of the checkpointing algorithm for generation of the forward solution during the integration of the adjoint system.

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 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:

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

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

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.

[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 [38].

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 $g(T, y(T))$). 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 [38] 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 [38] 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 [13].

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 Figs. 3.1 and 3.2). 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 3.3. The central integration module, implemented in the files `idas.h`, `idas_impl.h`, and `idas.c`, deals with the evaluation of integration coefficients, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues.

IDAS utilizes generic linear and nonlinear solver modules defined by the SUNLINSOL API (see Chapter 9) and SUNNONLINSOL API (see Chapter 10) respectively. As such, IDAS has no knowledge of the method being used to solve the linear and nonlinear systems that arise in each time step. For any given user problem, there exists a single nonlinear solver interface and, if necessary, one of the linear system solver interfaces is specified, and invoked as needed during the integration. While SUNDIALS includes a fixed-point nonlinear solver module, it is not currently supported in IDAS (note the fixed-point module is listed in Figure 3.1 but not Figure 3.3).

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

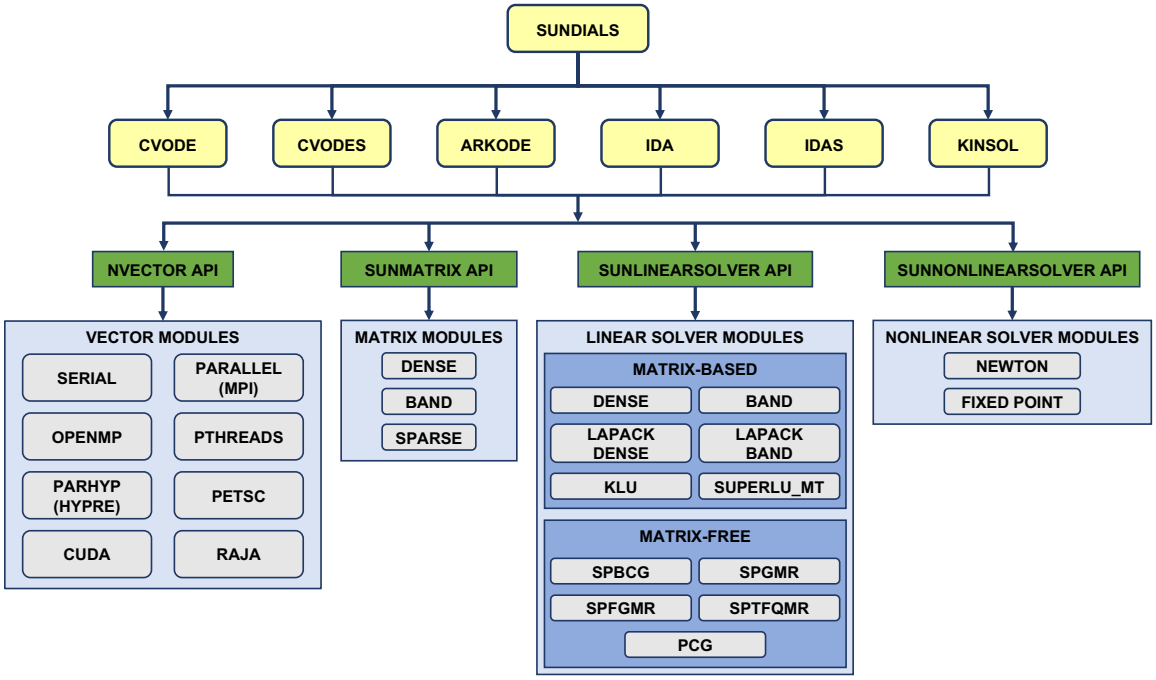


Figure 3.1: High-level diagram of the SUNDIALS suite

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

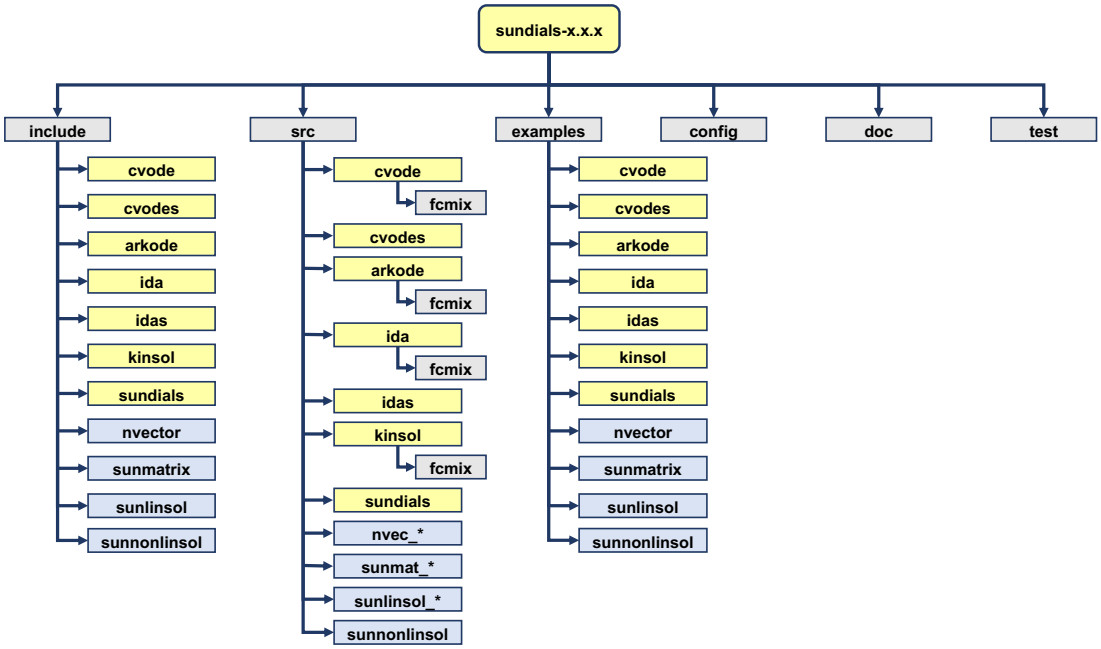
The adjoint sensitivity module (file `idaa.c`) provides the infrastructure needed for the backward integration of any system of DAEs which depends on the solution of the original IVP, in particular the adjoint system and any quadratures required in evaluating the gradient of the objective functional.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

IDAS now has a single unified linear solver interface, IDALS, supporting both direct and iterative linear solvers built using the generic SUNLINSOL API (see Chapter 9). These solvers may utilize a SUNMATRIX object (see Chapter 8) for storing Jacobian information, or they may be matrix-free. Since IDAS can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to IDAS will expand as new SUNLINSOL modules are developed.

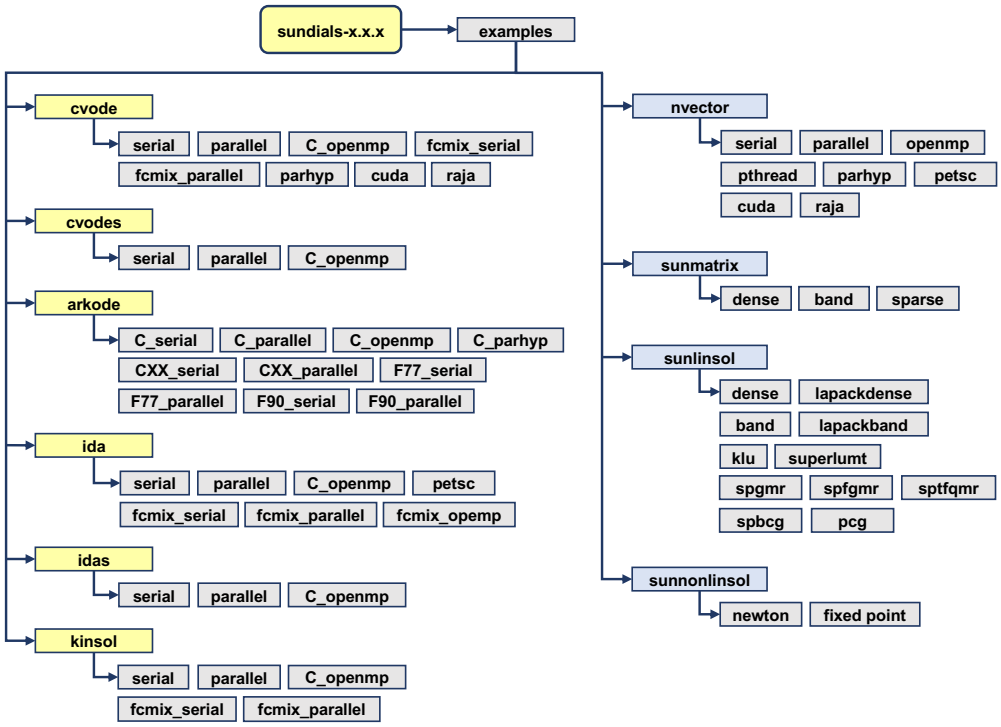
For users employing dense or banded Jacobian matrices, IDALS includes algorithms for their approximation through difference quotients, but the user also has the option of supplying the Jacobian (or an approximation to it) directly. This user-supplied routine is required when using sparse or user-supplied Jacobian matrices.

For users employing matrix-free iterative linear solvers, IDALS includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector, Jv. Again, the user has the option of providing routines for this operation, in two phases: setup (preprocessing of Jacobian data) and multiplication.

For preconditioned iterative methods, the preconditioning must be supplied by the user, again in two phases: setup and solve. While there is no default choice of preconditioner analogous to the difference-quotient approximation in the direct case, the references [6, 10], together with the example and demonstration programs included with IDAS, offer considerable assistance in building



(a) Directory structure of the SUNDIALS source tree



(b) Directory structure of the SUNDIALS examples

Figure 3.2: Organization of the SUNDIALS suite

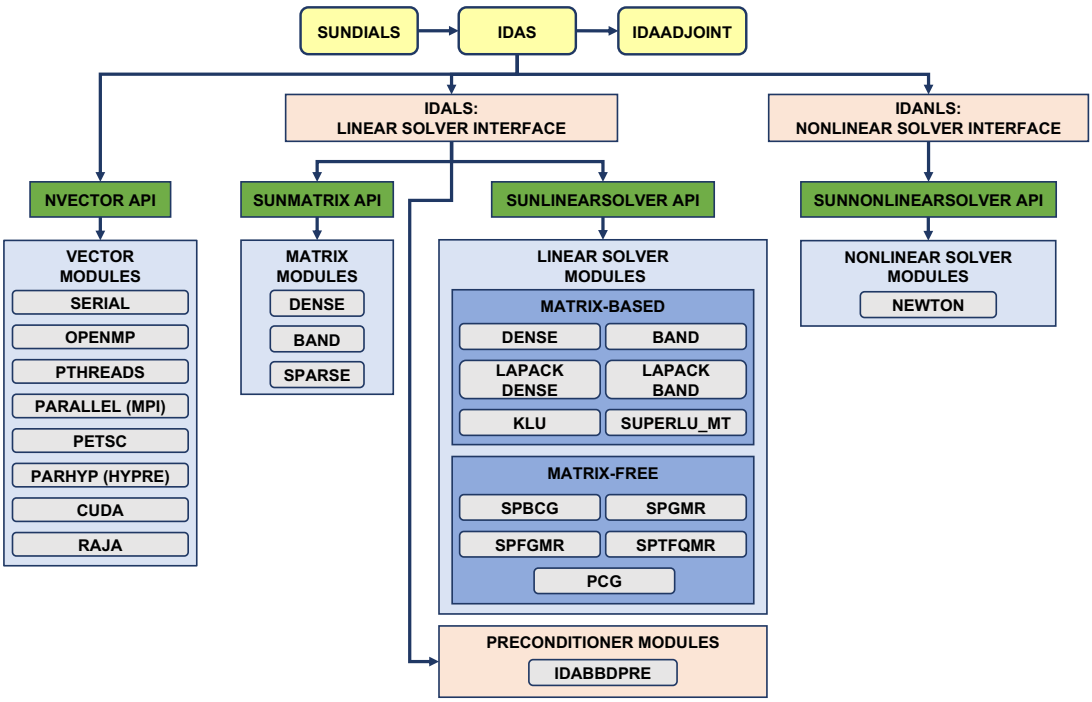


Figure 3.3: Overall structure diagram of the IDA package. Modules specific to IDA begin with "IDA" (IDALS, IDABBDPRE, and IDANLS), all other items correspond to generic solver and auxiliary modules. Note also that the LAPACK, KLU and SUPERLUMT support is through interfaces to external packages. Users will need to download and compile those packages independently.

preconditioners.

IDAS' linear solver interface consists of four primary routines, devoted to (1) memory allocation and initialization, (2) setup of the matrix data involved, (3) solution of the system, and (4) 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 four associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

IDAS also provides a preconditioner module, IDABBDPRE, for use with any of the Krylov iterative linear solvers. It works in conjunction with NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a banded 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 in a C language setting. 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 [30].

The sample programs described in the companion document [43] 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 SUNLINSOL and SUNMATRIX modules are compatible with all NVECTOR implementations. Details on compatibility are given in the documentation for each SUNMATRIX module (Chapter 8) and each SUNLINSOL module (Chapter 9). For example, NVECTOR_PARALLEL is not compatible with the dense, banded, or sparse SUNMATRIX types, or with the corresponding dense, banded, or sparse SUNLINSOL modules. Please check Chapters 8 and 9 to verify compatibility between these modules. In addition to that documentation, we note that the preconditioner module IDABBDPRE can only be used with NVECTOR_PARALLEL. 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.

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*,

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`
- *incdir*`/include/sunmatrix`

- *incdir*/include/sunlinsol
- *incdir*/include/sunnonlinsol

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 32- or 64-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 int32_t and int64_t with int and long 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/idas.h`, the header file for IDAS, which defines the several types and various constants, and includes function prototypes. This includes the header file for IDALS, `ida/ida_ls.h`.

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

The calling program must also include an NVECTOR implementation header file, of the form `nvector/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.

If using a non-default nonlinear solver module, or when interacting with a SUNNONLINSOL module directly, the calling program must also include a SUNNONLINSOL implementation header file, of the form `sunnonlinsol/sunnonlinsol_***.h` where `***` is the name of the nonlinear solver module (see Chapter 10 for more information). This file in turn includes the header file `sundials_nonlinearsolver.h` which defines the abstract `SUNNonlinearSolver` data type.

If using a nonlinear solver that requires the solution of a linear system of the form (2.5) (e.g., the default Newton iteration), a linear solver module header file is also required. The header files corresponding to the various SUNDIALS-provided linear solver modules available for use with IDAS are:

- Direct linear solvers:
  - `sunlinsol/sunlinsol_dense.h`, which is used with the dense linear solver module, SUNLINSOL_DENSE;
  - `sunlinsol/sunlinsol_band.h`, which is used with the banded linear solver module, SUNLINSOL_BAND;
  - `sunlinsol/sunlinsol_lapackdense.h`, which is used with the LAPACK dense linear solver module, SUNLINSOL_LAPACKDENSE;
  - `sunlinsol/sunlinsol_lapackband.h`, which is used with the LAPACK banded linear solver module, SUNLINSOL_LAPACKBAND;
  - `sunlinsol/sunlinsol_klu.h`, which is used with the KLU sparse linear solver module, SUNLINSOL_KLU;
  - `sunlinsol/sunlinsol_superlumt.h`, which is used with the SUPERLUMT sparse linear solver module, SUNLINSOL_SUPERLUMT;
- Iterative linear solvers:
  - `sunlinsol/sunlinsol_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver module, SUNLINSOL_SPGMR;
  - `sunlinsol/sunlinsol_spfgmr.h`, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, SUNLINSOL_SPFGMR;
  - `sunlinsol/sunlinsol_spbcgs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, SUNLINSOL_SPBCGS;

- `sunlinsol/sunlinsol_sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov linear solver module, SUNLINSOL_SPTFQMR;
- `sunlinsol/sunlinsol_pcg.h`, which is used with the scaled, preconditioned CG Krylov linear solver module, SUNLINSOL_PCG;

The header files for the SUNLINSOL_DENSE and SUNLINSOL_LAPACKDENSE linear solver modules include the file `sunmatrix/sunmatrix_dense.h`, which defines the SUNMATRIX_DENSE matrix module, as as well as various functions and macros acting on such matrices.

The header files for the SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND linear solver modules include the file `sunmatrix/sunmatrix_band.h`, which defines the SUNMATRIX_BAND matrix module, as as well as various functions and macros acting on such matrices.

The header files for the SUNLINSOL_KLU and SUNLINSOL_SUPERLUMT sparse linear solvers include the file `sunmatrix/sunmatrix_sparse.h`, which defines the SUNMATRIX_SPARSE matrix module, as well as various functions and macros acting on such matrices.

The header files for the Krylov iterative solvers include the file `sundials/sundials_iterative.h`, which enumerates the kind of preconditioning, and (for the SPGMR and SPFGMR solvers) 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 [43]), preconditioning is done with a block-diagonal matrix. For this, even though the SUNLINSOL_SPGMR linear solver is used, the header `sundials/sundials_dense.h` is included for access to the underlying generic dense matrix arithmetic routines.

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, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapter 7, 8, 9, and 10 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 §7.2-7.5 for details.

   For the *hypre* and PETSc vector wrappers, first create and initialize the underlying vector and then create an 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 §7.6 and §7.7 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 §7.8-7.9 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. **Create matrix object**

   If a nonlinear solver requiring a linear solver will be used (e.g., the default Newton iteration) and the linear solver will be a matrix-based linear solver, then a template Jacobian matrix must be created by using the appropriate constructor function defined by the particular SUNMATRIX implementation.

   For the SUNDIALS-supplied SUNMATRIX implementations, the matrix object may be created using a call of the form

   ```
   SUNMatrix J = SUNBandMatrix(...);
   ```

   or

   ```
   SUNMatrix J = SUNDenseMatrix(...);
   ```

   or

   ```
   SUNMatrix J = SUNSparseMatrix(...);
   ```

   NOTE: The dense, banded, and sparse matrix objects are usable only in a serial or threaded environment.

8. **Create linear solver object**

   If a nonlinear solver requiring a linear solver is chosen (e.g., the default Newton iteration), then the desired linear solver object must be created by calling the appropriate constructor function defined by the particular SUNLINSOL implementation.

   For any of the SUNDIALS-supplied SUNLINSOL implementations, the linear solver object may be created using a call of the form

   ```
   SUNLinearSolver LS = SUNLinSol_*(...);
   ```

   where `*` can be replaced with "Dense", "SPGMR", or other options, as discussed in §4.5.3 and Chapter 9.

9. **Set linear solver optional inputs**

   Call `*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See the documentation for each SUNLINSOL module in Chapter 9 for details.

10. **Attach linear solver module**

    If a nonlinear solver requiring a linear solver is chosen (e.g., the default Newton iteration), then initialize the IDALS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with the following call (for details see §4.5.3):

    `ier = IDASetLinearSolver(...);`

11. **Set optional inputs**

    Optionally, call `IDASet*` functions to change from their default values any optional inputs that control the behavior of IDAS. See §4.5.8.1 and §4.5.8 for details.

12. **Create nonlinear solver object** (*optional*)

    If using a non-default nonlinear solver (see §4.5.4), then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular SUNNONLINSOL implementation (e.g., `NLS = SUNNonlinSol_***(...);` where `***` is the name of the nonlinear solver (see Chapter 10 for details).

13. **Attach nonlinear solver module** (*optional*)

    If using a non-default nonlinear solver, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling `ier = IDASetNonlinearSolver(ida_mem, NLS);` (see §4.5.4 for details).

14. **Set nonlinear solver optional inputs** (*optional*)

    Call the appropriate set functions for the selected nonlinear solver module to change optional inputs specific to that nonlinear solver. These *must* be called after `IDAInit` if using the default nonlinear solver or after attaching a new nonlinear solver to IDAS, otherwise the optional inputs will be overridden by IDAS defaults. See Chapter 10 for more information on optional inputs.

15. **Correct initial values**

    Optionally, call `IDACalcIC` to correct the initial values `y0` and `yp0` passed to `IDAInit`. See §4.5.5. Also see §4.5.8.3 for relevant optional input calls.

16. **Specify rootfinding problem**

    Optionally, call `IDARootInit` to initialize a rootfinding problem to be solved during the integration of the DAE system. See §4.5.6 for details, and see §4.5.8.4 for relevant optional input calls.

17. **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` (which can be the same as the vector `yp0` above) will contain $\dot{y}(t)$. See §4.5.7 for details.

18. **Get optional outputs**

    Call `IDA*Get*` functions to obtain optional output. See §4.5.10 for details.

19. **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`.

20. **Free solver memory**

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

21. **Free nonlinear solver memory** (*optional*)

    If a non-default nonlinear solver was used, then call `SUNNonlinSolFree(NLS)` to free any memory allocated for the SUNNONLINSOL object.

22. **Free linear solver and matrix memory**

    Call `SUNLinSolFree` and `SUNMatDestroy` to free any memory allocated for the linear solver and matrix objects created above.

23. **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 §4.5.8, 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 §4.5.8.1).

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 [43]. 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 interface functions

As previously explained, if the nonlinear solver requires the solution of linear systems of the form (2.5) (e.g., the default Newton iteration, then solution of these linear systems is handled with the IDALS linear solver interface. This interface supports all valid SUNLINSOL modules. Here, matrix-based SUNLINSOL modules utilize SUNMATRIX objects to store the Jacobian matrix $J = \partial F/\partial y + \alpha \partial F/\partial \dot{y}$ and factorizations used throughout the solution process. Conversely, matrix-free SUNLINSOL modules instead use iterative methods to solve the linear systems of equations, and only require the *action* of the Jacobian on a vector, Jv.

With most iterative linear solvers, preconditioning can be done on the left only, on the right only, on both the left and the right, or not at all. The exceptions to this rule are SPFGMR that supports

right preconditioning only and PCG that performs symmetric preconditioning. However, in IDAS only left preconditioning is supported. For the specification of a preconditioner, see the iterative linear solver sections in §4.5.8 and §4.6. A preconditioner matrix P must approximate the Jacobian J, at least crudely.

To specify a generic linear solver to IDAS, after the call to `IDACreate` but before any calls to `IDASolve`, the user's program must create the appropriate SUNLINSOL object and call the function `IDASetLinearSolver`, as documented below. To create the `SUNLinearSolver` object, the user may call one of the SUNDIALS-packaged SUNLINSOL module constructor routines via a call of the form

```
SUNLinearSolver LS = SUNLinSol_*(...);
```

The current list of such constructor routines includes `SUNLinSol_Dense`, `SUNLinSol_Band`, `SUNLinSol_LapackDense`, `SUNLinSol_LapackBand`, `SUNLinSol_KLU`, `SUNLinSol_SuperLUMT`, `SUNLinSol_SPGMR`, `SUNLinSol_SPFGMR`, `SUNLinSol_SPBCGS`, `SUNLinSol_SPTFQMR`, and `SUNLinSol_PCG`.

Alternately, a user-supplied `SUNLinearSolver` module may be created and used instead. The use of each of the generic linear solvers involves certain constants, functions 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 specific SUNMATRIX or SUNLINSOL module in question, as described in Chapters 8 and 9.

Once this solver object has been constructed, the user should attach it to IDAS via a call to `IDASetLinearSolver`. The first argument passed to this function is the IDAS memory pointer returned by `IDACreate`; the second argument is the desired SUNLINSOL object to use for solving systems. The third argument is an optional SUNMATRIX object to accompany matrix-based SUNLINSOL inputs (for matrix-free linear solvers, the third argument should be `NULL`). A call to this function initializes the IDALS linear solver interface, linking it to the main IDAS integrator, and allows the user to specify additional parameters and routines pertinent to their choice of linear solver.

`IDASetLinearSolver`

Call `flag = IDASetLinearSolver(ida_mem, LS, J);`

Description The function `IDASetLinearSolver` attaches a generic SUNLINSOL object `LS` and corresponding template Jacobian SUNMATRIX object `J` (if applicable) to IDAS, initializing the IDALS linear solver interface.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `LS` (`SUNLinearSolver`) SUNLINSOL object to use for solving linear systems of the form (2.5.
- `J` (`SUNMatrix`) SUNMATRIX object for used as a template for the Jacobian (or `NULL` if not applicable).

Return value The return value `flag` (of type `int`) is one of
- `IDALS_SUCCESS` The IDALS initialization was successful.
- `IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDALS_ILL_INPUT` The IDALS interface is not compatible with the `LS` or `J` input objects or is incompatible with the current NVECTOR module.
- `IDALS_SUNLS_FAIL` A call to the `LS` object failed.
- `IDALS_MEM_FAIL` A memory allocation request failed.

Notes If `LS` is a matrix-based linear solver, then the template Jacobian matrix `J` will be used in the solve process, so if additional storage is required within the SUNMATRIX object (e.g., for factorization of a banded matrix), ensure that the input object is allocated with sufficient size (see the documentation of the particular SUNMATRIX type in Chapter 8 for further information).

The previous routines `IDADlsSetLinearSolver` and `IDASpilsSetLinearSolver` are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

4.5.4 Nonlinear solver interface function

By default IDAS uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §10.2). To specify a different nonlinear solver in IDAS, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to IDAS by calling `IDASetNonlinearSolver`, as documented below.

When changing the nonlinear solver in IDAS, `IDASetNonlinearSolver` must be called after `IDAInit`. If any calls to `IDASolve` have been made, then IDAS will need to be reinitialized by calling `IDAReInit` to ensure that the nonlinear solver is initialized correctly before any subsequent calls to `IDASolve`.

The first argument passed to the routine `IDASetNonlinearSolver` is the IDAS memory pointer returned by `IDACreate` and the second argument is the SUNNONLINSOL object to use for solving the nonlinear system 2.4. A call to this function attaches the nonlinear solver to the main IDAS integrator. We note that at present, the SUNNONLINSOL object *must be of type* `SUNNONLINEARSOLVER_ROOTFIND`.

`IDASetNonlinearSolver`

Call `flag = IDASetNonlinearSolver(ida_mem, NLS);`

Description The function `IDASetNonLinearSolver` attaches a SUNNONLINSOL object (`NLS`) to IDAS.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `NLS` (`SUNNonlinearSolver`) SUNNONLINSOL object to use for solving nonlinear systems.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The nonlinear solver was successfully attached.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDA_ILL_INPUT` The SUNNONLINSOL object is `NULL`, does not implement the required nonlinear solver operations, is not of the correct type, or the residual function, convergence test function, or maximum number of nonlinear iterations could not be set.

Notes When forward sensitivity analysis capabilities are enabled and the `IDA_STAGGERED` corrector method is used this function sets the nonlinear solver method for correcting state variables (see §5.2.3 for more details).

4.5.5 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. [8].) 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 §4.5.10.3).

4.5.6 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`$= 0$.

4.5.7 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 §4.5.10.4 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.

4.5.8 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.

4.5.8.1 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.

Table 4.2: Optional inputs for IDAS and IDALS

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`	`SUNFALSE`
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`	`SUNFALSE`
Lower bound on Newton step	`IDASetStepToleranceIC`	$\text{uround}^{2/3}$
IDALS linear solver interface		
Jacobian function	`IDASetJacFn`	DQ
Jacobian-times-vector function	`IDASetJacTimes`	NULL, DQ
Preconditioner functions	`IDASetPreconditioner`	NULL, NULL
Ratio between linear and nonlinear tolerances	`IDASetEpsLin`	0.05
Increment factor used in DQ Jv approx.	`IDASetIncrementFactor`	1.0

`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.
`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 $|h| \leq .001|\texttt{tout - t0}|$.

`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.

IDA_MEM_FAIL The SUNNONLINSOL module 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 (`SUNTRUE`) or not (`SUNFALSE`) 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 `SUNFALSE`.

If `suppressalg`=`SUNTRUE` 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 = SUNTRUE`) 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. [4] 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 §4.5.5).

`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 or the simultaneous corrector option has been selected when doing forward sensitivity analysis.

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.

Constraint checking when doing forward sensitivity analysis with the simultaneous corrector option is currently disallowed and will result in an illegal input return.

4.5.8.2 Linear solver interface optional input functions

The mathematical explanation of the linear solver methods available to IDAS is provided in §2.1. We group the user-callable routines into four categories: general routines concerning the overall IDALS linear solver interface, optional inputs for matrix-based linear solvers, optional inputs for matrix-free linear solvers, and optional inputs for iterative linear solvers. We note that the matrix-based and matrix-free groups are mutually exclusive, whereas the "iterative" tag can apply to either case.

When using matrix-based linear solver modules, the IDALS solver interface needs a function to compute an approximation to the Jacobian matrix $J(t, y, \dot{y})$. This function must be of type `IDALsJacFn`. The user can supply a Jacobian function, or if using a dense or banded matrix J can use the default internal difference quotient approximation that comes with the IDALS interface. To specify a user-supplied Jacobian function `jac`, IDALS provides the function `IDASetJacFn`. The IDALS interface

passes the pointer `user_data` to the 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`.

`IDASetJacFn`

Call `flag = IDASetJacFn(ida_mem, jac);`

Description The function `IDASetJacFn` specifies the Jacobian approximation function to be used for a matrix-based solver within the IDALS interface.

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

Return value The return value `flag` (of type `int`) is one of
`IDALS_SUCCESS` The optional value has been successfully set.
`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.
`IDALS_LMEM_NULL` The IDALS linear solver interface has not been initialized.

Notes This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.

By default, IDALS uses an internal difference quotient function for dense and band matrices. If `NULL` is passed to `jac`, this default function is used. An error will occur if no `jac` is supplied when using other matrix types.

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

The previous routine `IDADlsSetJacFn` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

When using matrix-free linear solver modules, the IDALS solver interface requires a function to compute an approximation to the product between the Jacobian matrix $J(t, y)$ and a vector v. The user can supply a Jacobian-times-vector approximation function, or use the default internal difference quotient function that comes with the IDALS solver interface. A user-defined Jacobian-vector function must be of type `IDALsJacTimesVecFn` and can be specified through a call to `IDASetJacTimes` (see §4.6.6 for specification details). The evaluation and processing of any Jacobian-related data needed by the user's Jacobian-times-vector function may be done in the optional user-supplied function `jtsetup` (see §4.6.7 for specification details). The pointer `user_data` received through `IDASetUserData` (or a pointer to `NULL` if `user_data` was not specified) is passed to the Jacobian-times-vector setup and product functions, `jtsetup` and `jtimes`, each time they are called. 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.

`IDASetJacTimes`

Call `flag = IDASetJacTimes(ida_mem, jsetup, jtimes);`

Description The function `IDASetJacTimes` specifies the Jacobian-vector setup and product functions.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`jtsetup` (`IDALsJacTimesSetupFn`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.
`jtimes` (`IDALsJacTimesVecFn`) user-defined Jacobian-vector product function.

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

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_SUNLS_FAIL An error occurred when setting up the system matrix-times-vector routines in the SUNLINSOL object used by the IDALS interface.

Notes The default is to use an internal finite difference quotient for `jtimes` and to omit `jtsetup`. If `NULL` is passed to `jtimes`, these defaults are used. A user may specify non-`NULL` `jtimes` and `NULL` `jtsetup` inputs.

This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.

The function type `IDALsJacTimesSetupFn` is described in §4.6.7.

The function type `IDALsJacTimesVecFn` is described in §4.6.6.

The previous routine `IDASpilsSetJacTimes` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

Alternately, when using the default difference-quotient approximation to the Jacobian-vector product, the user may specify the factor to use in setting increments for the finite-difference approximation, via a call to `IDASetIncrementFactor`:

`IDASetIncrementFactor`

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

Description The function `IDASetIncrementFactor` specifies the increment factor to be used in the difference-quotient approximation to the product Jv. Specifically, Jv is approximated via the formula

$$Jv = \frac{1}{\sigma}\left[F(t, \tilde{y}, \tilde{y}') - F(t, y, y')\right],$$

where $\tilde{y} = y + \sigma v$, $\tilde{y}' = y' + c_j \sigma v$, c_j is a BDF parameter proportional to the step size, $\sigma = \sqrt{N}$ `dqincfac`, and N is the number of equations in the DAE system.

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

`dqincfac` (`realtype`) user-specified increment factor (positive).

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

IDALS_SUCCESS The optional value has been successfully set.

IDALS_MEM_NULL The `ida_mem` pointer is `NULL`.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_ILL_INPUT The specified value of `dqincfac` is ≤ 0.

Notes The default value is 1.0.

This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.

The previous routine `IDASpilsSetIncrementFactor` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

When using an iterative linear solver, the user may supply a preconditioning operator to aid in solution of the system. This operator consists of two user-supplied functions, `psetup` and `psolve`, that are supplied to IDA using the function `IDASetPreconditioner`. The `psetup` function supplied to this routine should handle evaluation and preprocessing of any Jacobian data needed by the user's preconditioner solve function, `psolve`. Both of these functions are fully specified in §4.6. The user data pointer received through `IDASetUserData` (or a pointer to `NULL` if user data was not specified) is passed to the `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.

Also, as described in §2.1, the IDALS interface requires that iterative linear solvers stop when the norm of the preconditioned residual satisfies

$$\|r\| \leq \frac{\epsilon_L \epsilon}{10}$$

where ϵ is the nonlinear solver tolerance, and the default $\epsilon_L = 0.05$; this value may be modified by the user through the `IDASetEpsLin` function.

`IDASetPreconditioner`

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

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

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

`psetup` (`IDALsPrecSetupFn`) user-defined function to set up the preconditioner. Pass `NULL` if no setup is necessary.

`psolve` (`IDALsPrecSolveFn`) user-defined preconditioner solve function.

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

`IDALS_SUCCESS` The optional values have been successfully set.

`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.

`IDALS_SUNLS_FAIL` An error occurred when setting up preconditioning in the SUNLINSOL object used by the IDALS interface.

Notes The default is `NULL` for both arguments (i.e., no preconditioning).

This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.

The function type `IDALsPrecSolveFn` is described in §4.6.8.

The function type `IDALsPrecSetupFn` is described in §4.6.9.

The previous routine `IDASpilsSetPreconditioner` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDASetEpsLin`

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

Description The function `IDASetEpsLin` specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the nonlinear iteration test constant.

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

`IDALS_SUCCESS` The optional value has been successfully set.

`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.

`IDALS_ILL_INPUT` The factor `eplifac` is negative.

Notes The default value is 0.05.

This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.

If `eplifac`$= 0.0$ is passed, the default value is used.

The previous routine IDASpilsSetEpsLin is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

4.5.8.3 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 IDAS 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 (SUNTRUE) or keep (SUNFALSE) 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 SUNFALSE.

`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)$^{2/3}$.

4.5.8.4 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.

4.5.9 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 §4.5.10.2) can be used to access t_n, h_u and $klast$.

4.5.10 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 nonlinear solver 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 matrix-based 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.

4.5.10.1 SUNDIALS version information

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

Table 4.3: Optional outputs from IDAS and IDALS

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
IDALS linear solver interface	
Size of real and integer workspace	IDAGetLinWorkSpace
No. of Jacobian evaluations	IDAGetNumJacEvals
No. of residual calls for finite diff. Jacobian[-vector] evals.	IDAGetNumLinResEvals
No. of linear iterations	IDAGetNumLinIters
No. of linear convergence failures	IDAGetNumLinConvFails
No. of preconditioner evaluations	IDAGetNumPrecEvals
No. of preconditioner solves	IDAGetNumPrecSolves
No. of Jacobian-vector setup evaluations	IDAGetNumJTSetupEvals
No. of Jacobian-vector product evaluations	IDAGetNumJtimesEvals
Last return from a linear solver function	IDAGetLastLinFlag
Name of constant associated with a return flag	IDAGetLinReturnFlagName

`SUNDIALSGetVersion`

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

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

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

Return value If successful, `SUNDIALSGetVersion` returns 0 and `version` contains the SUNDIALS version information. Otherwise, it returns -1 and `version` is not set (the input character array is too short).

Notes A string of 25 characters should be sufficient to hold the version information. Any trailing characters in the `version` array are removed.

`SUNDIALSGetVersionNumber`

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

Description The function `SUNDIALSGetVersionNumber` set integers for the SUNDIALS major, minor, and patch release numbers and fills a character array 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 *`) character array to hold the SUNDIALS release label.
`len` (`int`) allocated length of the `label` character array.

Return value If successful, `SUNDIALSGetVersionNumber` returns 0 and the `major`, `minor`, `patch`, and `label` values are set. Otherwise, it returns -1 and the values are not set (the input character array is too short).

Notes A string of 10 characters should be sufficient to hold the label information. If a label is not used in the release version, no information is copied to `label`. Any trailing characters in the `label` array are removed.

4.5.10.2 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 SUNNONLINSOL 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 §4.5.6), 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 $m = \max($`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 IDAS, 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 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.
IDA_MEM_FAIL	The SUNNONLINSOL module 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.

IDA_MEM_FAIL The SUNNONLINSOL module 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.

4.5.10.3 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).

4.5.10.4 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`.

4.5.10.5 IDALS linear solver interface optional output functions

The following optional outputs are available from the IDALS modules: workspace requirements, number of calls to the Jacobian routine, number of calls to the residual routine for finite-difference Jacobian or Jacobian-vector product approximation, 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 setup and product routines, and last return value from an IDALS 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 (e.g., `lenrwLS`).

`IDAGetLinWorkSpace`

Call `flag = IDAGetLinWorkSpace(ida_mem, &lenrwLS, &leniwLS);`

Description The function `IDAGetLinWorkSpace` returns the sizes of the real and integer workspaces used by the IDALS linear solver interface.

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

`lenrwLS` (`long int`) the number of real values in the IDALS workspace.

`leniwLS` (`long int`) the number of integer values in the IDALS workspace.

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

`IDALS_SUCCESS` The optional output value has been successfully set.

`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.

Notes The workspace requirements reported by this routine correspond only to memory allocated within this interface and to memory allocated by the SUNLINSOL object attached to it. The template Jacobian matrix allocated by the user outside of IDALS is not included in this report.

The previous routines `IDADlsGetWorkspace` and `IDASpilsGetWorkspace` are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetNumJacEvals`

Call `flag = IDAGetNumJacEvals(ida_mem, &njevals);`

Description The function `IDAGetNumJacEvals` returns the cumulative number of calls to the IDALS 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

`IDALS_SUCCESS`	The optional output value has been successfully set.
`IDALS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDALS_LMEM_NULL`	The IDALS linear solver has not been initialized.

Notes The previous routine `IDADlsGetNumJacEvals` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetNumLinResEvals`

Call `flag = IDAGetNumLinResEvals(ida_mem, &nrevalsLS);`

Description The function `IDAGetNumLinResEvals` returns the cumulative number of calls to the user residual function due to the finite difference Jacobian approximation or 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

`IDALS_SUCCESS`	The optional output value has been successfully set.
`IDALS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDALS_LMEM_NULL`	The IDALS linear solver has not been initialized.

Notes The value `nrevalsLS` is incremented only if one of the default internal difference quotient functions is used.

The previous routines `IDADlsGetNumRhsEvals` and `IDASpilsGetNumRhsEvals` are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetNumLinIters`

Call `flag = IDAGetNumLinIters(ida_mem, &nliters);`

Description The function `IDAGetNumLinIters` 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

IDALS_SUCCESS The optional output value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

Notes The previous routine IDASpilsGetNumLinIters is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDAGetNumLinConvFails

Call flag = IDAGetNumLinConvFails(ida_mem, &nlcfails);

Description The function IDAGetNumLinConvFails 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

IDALS_SUCCESS The optional output value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

Notes The previous routine IDASpilsGetNumConvFails is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDAGetNumPrecEvals

Call flag = IDAGetNumPrecEvals(ida_mem, &npevals);

Description The function IDAGetNumPrecEvals 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

IDALS_SUCCESS The optional output value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

Notes The previous routine IDASpilsGetNumPrecEvals is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDAGetNumPrecSolves

Call flag = IDAGetNumPrecSolves(ida_mem, &npsolves);

Description The function IDAGetNumPrecSolves 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

IDALS_SUCCESS The optional output value has been successfully set.

`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.

Notes The previous routine `IDASpilsGetNumPrecSolves` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetNumJTSetupEvals`

Call `flag = IDAGetNumJTSetupEvals(ida_mem, &njtsetup);`

Description The function `IDAGetNumJTSetupEvals` returns the cumulative number of calls made to the Jacobian-vector setup function `jtsetup`.

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

`njtsetup` (`long int`) the current number of calls to `jtsetup`.

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_LMEM_NULL` The IDA linear solver has not been initialized.

Notes The previous routine `IDASpilsGetNumJTSetupEvals` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetNumJtimesEvals`

Call `flag = IDAGetNumJtimesEvals(ida_mem, &njvevals);`

Description The function `IDAGetNumJtimesEvals` 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

`IDA_SUCCESS` The optional output value has been successfully set.

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

`IDA_LMEM_NULL` The IDA linear solver has not been initialized.

Notes The previous routine `IDASpilsGetNumJtimesEvals` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetLastLinFlag`

Call `flag = IDAGetLastLinFlag(ida_mem, &lsflag);`

Description The function `IDAGetLastLinFlag` returns the last return value from an IDALS routine.

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

`lsflag` (`long int`) the value of the last return flag from an IDALS function.

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

`IDALS_SUCCESS` The optional output value has been successfully set.

`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.

`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.

Notes If the IDALS setup function failed (i.e., `IDASolve` returned `IDA_LSETUP_FAIL`) when using the SUNLINSOL_DENSE or SUNLINSOL_BAND modules, then the value of `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 banded) Jacobian matrix.

If the IDALS setup function failed when using another SUNLINSOL module, then `lsflag` will be `SUNLS_PSET_FAIL_UNREC`, `SUNLS_ASET_FAIL_UNREC`, or `SUNLS_PACKAGE_FAIL_UNREC`.

If the IDALS solve function failed (`IDASolve` returned `IDA_LSOLVE_FAIL`), `lsflag` contains the error return flag from the SUNLINSOL object, which will be one of:
`SUNLS_MEM_NULL`, indicating that the SUNLINSOL memory is `NULL`;
`SUNLS_ATIMES_FAIL_UNREC`, indicating an unrecoverable failure in the $J * v$ function;
`SUNLS_PSOLVE_FAIL_UNREC`, indicating that the preconditioner solve function `psolve` failed unrecoverably; `SUNLS_GS_FAIL`, indicating a failure in the Gram-Schmidt procedure (generated only in SPGMR or SPFGMR); `SUNLS_QRSOL_FAIL`, indicating that the matrix R was found to be singular during the QR solve phase (SPGMR and SPFGMR only); or `SUNLS_PACKAGE_FAIL_UNREC`, indicating an unrecoverable failure in an external iterative linear solver package.

The previous routines `IDADlsGetLastFlag` and `IDASpilsGetLastFlag` are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

`IDAGetLinReturnFlagName`

Call `name = IDAGetLinReturnFlagName(lsflag);`

Description The function `IDAGetLinReturnFlagName` returns the name of the IDA constant corresponding to `lsflag`.

Arguments The only argument, of type `long int`, is a return flag from an IDALS function.

Return value The return value is a string containing the name of the corresponding constant.

If $1 \le$ `lsflag` $\le N$ (LU factorization failed), this function returns "NONE".

Notes The previous routines `IDADlsGetReturnFlagName` and `IDASpilsGetReturnFlagName` are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

4.5.11 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 calls to either the linear solver objects themselves, or to the IDALS interface routines, as described in §4.5.3.

If there are changes to any optional inputs, make the appropriate `IDASet***` calls, as described in §4.5.8. 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) one or two functions that provide Jacobian-related information for the linear solver, 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 nonlinear solve, 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 construction (matrix-based linear solvers)

If a matrix-based linear solver module is used (i.e. a non-`NULL` SUNMATRIX object was supplied to `IDASetLinearSolver`), the user may provide a function of type `IDALsJacFn` defined as follows:

`IDALsJacFn`

Definition
```
typedef int (*IDALsJacFn)(realtype tt, realtype cj,
                          N_Vector yy, N_Vector yp, N_Vector rr,
                          SUNMatrix Jac, void *user_data,
                          N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the Jacobian matrix J of the DAE system (or an approximation to it), defined by Eq. (2.6).

Arguments

`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 (of type `SUNMatrix`), $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$.
`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 `IDALsJacFn` function as temporary storage or work space.

Return value An `IDALsJacFn` 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 Information regarding the structure of the specific SUNMATRIX structure (e.g., number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 8 for details).

Prior to calling the user-supplied Jacobian function, the Jacobian matrix $J(t, y)$ is zeroed out, so only nonzero elements need to be loaded into `Jac`.

If the user's `IDALsJacFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These quantities may 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 §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

dense:
A user-supplied dense Jacobian function must load the `Neq` × `Neq` dense matrix `Jac` with an approximation to the Jacobian matrix $J(t, y, \dot{y})$ at the point (`tt`, `yy`, `yp`). The accessor macros `SM_ELEMENT_D` and `SM_COLUMN_D` allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the SUNMATRIX_DENSE type. `SM_ELEMENT_D(J, i, j)` references the (`i`, `j`)-th element of the dense matrix `Jac` (with `i`, `j` $= 0 \ldots$ `N` $- 1$). This macro is meant for small problems for which efficiency of access is not a major concern. Thus, in terms of the indices m and n ranging from 1 to N, the Jacobian element $J_{m,n}$ can be set using the statement `SM_ELEMENT_D(J, m-1, n-1)` = $J_{m,n}$. Alternatively, `SM_COLUMN_D(J, j)` returns a pointer to the first element of the `j`-th column of `Jac` (with `j` $= 0 \ldots$ `N` $- 1$), and the elements of the `j`-th column can then be accessed using ordinary array indexing. Consequently, $J_{m,n}$ can be loaded using the statements `col_n = SM_COLUMN_D(J, n-1);` `col_n[m-1]` = $J_{m,n}$. For large problems, it is more efficient to use `SM_COLUMN_D` than to use `SM_ELEMENT_D`. Note that both of these macros number rows and columns starting from 0. The SUNMATRIX_DENSE type and accessor macros are documented in §8.2.

banded:
A user-supplied banded Jacobian function must load the `Neq` × `Neq` banded matrix `Jac` with an approximation to the Jacobian matrix $J(t, y, \dot{y})$ at the point (`tt`, `yy`, `yp`). The accessor macros `SM_ELEMENT_B`, `SM_COLUMN_B`, and `SM_COLUMN_ELEMENT_B` allow the

user to read and write banded matrix elements without making specific references to the underlying representation of the SUNMATRIX_BAND type. SM_ELEMENT_B(J, i, j) references the (i, j)-th element of the banded matrix Jac, counting from 0. This macro is meant for use in small problems for which efficiency of access is not a major concern. Thus, in terms of the indices m and n ranging from 1 to N with (m, n) within the band defined by mupper and mlower, the Jacobian element $J_{m,n}$ can be loaded using the statement SM_ELEMENT_B(J, m-1, n-1) = $J_{m,n}$. The elements within the band are those with -mupper $\leq$ m-n $\leq$ mlower. Alternatively, SM_COLUMN_B(J, 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 i-th element of the j-th column is given by SM_COLUMN_ELEMENT_B(col_j, i, j), counting from 0. Thus, for (m, n) within the band, $J_{m,n}$ can be loaded by setting col_n = SM_COLUMN_B(J, n-1); and SM_COLUMN_ELEMENT_B(col_n, m-1, n-1) = $J_{m,n}$. The elements of the j-th column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type SUNMATRIX_BAND. The array col_n can be indexed from $-$mupper to mlower. For large problems, it is more efficient to use SM_COLUMN_B and SM_COLUMN_ELEMENT_B than to use the SM_ELEMENT_B macro. As in the dense case, these macros all number rows and columns starting from 0. The SUNMATRIX_BAND type and accessor macros are documented in §8.3.

sparse:
A user-supplied sparse Jacobian function must load the Neq $\times$ Neq compressed-sparse-column or compressed-sparse-row matrix Jac with an approximation to the Jacobian matrix $J(t, y, \dot{y})$ at the point (tt, yy, 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 index arrays as needed. The amount of allocated space in a SUNMATRIX_SPARSE object may be accessed using the macro SM_NNZ_S or the routine SUNSparseMatrix_NNZ. The SUNMATRIX_SPARSE type and accessor macros are documented in §8.4.

The previous function type IDADlsJacFn is identical to IDALsJacFn, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

4.6.6 Jacobian-vector product (matrix-free linear solvers)

If a matrix-free linear solver is to be used (i.e., a NULL-valued SUNMATRIX was supplied to IDASetLinearSolver), the user may provide a function of type IDALsJacTimesVecFn in the following form, to compute matrix-vector products Jv. If such a function is not supplied, the default is a difference quotient approximation to these products.

IDALsJacTimesVecFn

Definition
```
typedef int (*IDALsJacTimesVecFn)(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 `IDALsJacTimesVecFn` as temporary storage or work space.

Return value The value returned by the Jacobian-times-vector function should be 0 if successful. A nonzero value indicates that a nonrecoverable error occurred.

Notes This function must return a value of $J * v$ that uses the *current* value of J, i.e. as evaluated at the current $(t, y, \dot{y})$.

If the user's `IDALsJacTimesVecFn` 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 §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `IDASpilsJacTimesVecFn` is identical to `IDALsJacTimesVecFn`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

4.6.7 Jacobian-vector product setup (matrix-free linear solvers)

If the user's Jacobian-times-vector requires that any Jacobian-related data be preprocessed or evaluated, then this needs to be done in a user-supplied function of type `IDALsJacTimesSetupFn`, defined as follows:

`IDAJacTimesSetupFn`

Definition
```
typedef int (*IDAJacTimesSetupFn)(realtype tt, N_Vector yy,
                                  N_Vector yp, N_Vector rr,
                                  realtype cj, void *user_data);
```

Purpose This function preprocesses and/or evaluates Jacobian data needed by the Jacobian-times-vector routine.

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 $F(t, y, \dot{y})$.
`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`.

Return value The value returned by the Jacobian-vector setup function 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).

Notes Each call to the Jacobian-vector setup function is preceded by a call to the `IDAResFn` user function with the same `(t,y, yp)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual.

If the user's IDALsJacTimesVecFn 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 §4.5.10.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

The previous function type IDASpilsJacTimesSetupFn is identical to IDALsJacTimesSetupFn, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

4.6.8 Preconditioner solve (iterative linear solvers)

If a user-supplied preconditioner is to be used with a SUNLINSOL solver module, then the user must provide a 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 IDALsPrecSolveFn, defined as follows:

IDALsPrecSolveFn

Definition
```
typedef int (*IDALsPrecSolveFn)(realtype tt, N_Vector yy,
                                N_Vector yp, N_Vector rr,
                                N_Vector rvec, N_Vector zvec,
                                realtype cj, realtype delta,
                                void *user_data);
```

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 §4.5.10.2).
user_data	is a pointer to user data, the same as the user_data parameter passed to the function IDASetUserData.

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).

Notes The previous function type IDASpilsPrecSolveFn is identical to IDALsPrecSolveFn, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

4.6.9 Preconditioner setup (iterative linear solvers)

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 function of type IDALsPrecSetupFn, defined as follows:

`IDALsPrecSetupFn`

Definition
```
typedef int (*IDALsPrecSetupFn)(realtype tt, N_Vector yy,
                                N_Vector yp, N_Vector rr,
                                realtype cj, void *user_data);
```

Purpose This function evaluates and/or preprocesses Jacobian-related data needed by the preconditioner.

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 $F(t, y, \dot{y})$.
- `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`.

Return value The value 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 nonlinear solver.

If the user's `IDALsPrecSetupFn` 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 §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `IDASpilsPrecSetupFn` is identical to `IDALsPrecSetupFn`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

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 $(d/dt)\mathtt{yQ} = f_Q(t, y, \dot{y})$. 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. **Initialize IDAS solver**
6. **Specify integration tolerances**
7. **Create matrix object**
8. **Create linear solver object**
9. **Set linear solver optional inputs**
10. **Attach linear solver module**
11. **Set optional inputs**
12. **Create nonlinear solver object**
13. **Attach nonlinear solver module**
14. **Set nonlinear solver optional inputs**
15. **Correct initial values**
16. **Set vector of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.

17. **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.

18. **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.

19. **Advance solution in time**
20. **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.

21. **Get optional outputs**
22. **Get quadrature optional outputs**

    Call `IDAGetQuad*` functions to obtain optional output related to the integration of quadratures. See §4.7.5 for details.

23. **Deallocate memory for solution vectors and for the vector of quadrature variables**
24. **Free solver memory**

25. **Free nonlinear solver memory**

26. **Free linear solver and matrix memory**

27. **Finalize MPI, if used**

`IDAQuadInit` can be called and quadrature-related optional inputs (step 18 above) can be set, anywhere between steps 4 and 19.

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 §4.5.7. 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 (`SUNTRUE`) or not (`SUNFALSE`) 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 `SUNFALSE`.

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 = SUNTRUE`), `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 §7.2 and §7.3).

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 [32] 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 etc.**
3. **Set vectors of initial values**
4. **Create IDAS object**
5. **Initialize IDAS solver**
6. **Specify integration tolerances**
7. **Create linear solver object**

   When creating the iterative linear solver object, specify the use of left preconditioning (`PREC_LEFT`) as IDAS only supports left preconditioning.
8. **Set linear solver optional inputs**

9. **Attach linear solver module**

10. **Set optional inputs**

    Note that the user should not overwrite the preconditioner setup function or solve function through calls to idIDASetPreconditioner optional input function.

11. **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.

12. **Create nonlinear solver object**

13. **Attach nonlinear solver module**

14. **Set nonlinear solver optional inputs**

15. **Correct initial values**

16. **Specify rootfinding problem**

17. **Advance solution in time**

18. **Get optional outputs**

    Additional optional outputs associated with IDABBDPRE are available by way of two routines described below, `IDABBDPrecGetWorkSpace` and `IDABBDPrecGetNumGfnEvals`.

19. **Deallocate memory for solution vectors**

20. **Free solver memory**

21. **Free nonlinear solver memory**

22. **Free linear solver memory**

23. **Finalize MPI**

The user-callable functions that initialize (step 11 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

`IDALS_SUCCESS` The call to `IDABBDPrecInit` was successful.

`IDALS_MEM_NULL` The `ida_mem` pointer was `NULL`.

`IDALS_MEM_FAIL` A memory allocation request has failed.

`IDALS_LMEM_NULL` An IDALS linear solver memory was not attached.

`IDALS_ILL_INPUT` The supplied vector implementation was not compatible with the 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 the same linear solver choice, 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`. If there is a change in any of the linear solver inputs, an additional call to the "Set" routines provided by the SUNLINSOL module, and/or one or more of the corresponding `IDASet***` functions, must also be made (in the proper order).

`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

`IDALS_SUCCESS` The call to `IDABBDPrecReInit` was successful.

`IDALS_MEM_NULL` The `ida_mem` pointer was `NULL`.

IDALS_LMEM_NULL An IDALS linear solver memory was not attached.

IDALS_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

IDALS_SUCCESS The optional output value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer was NULL.

IDALS_PMEM_NULL The IDABBDPRE preconditioner has not been initialized.

Notes The workspace requirements reported by this routine correspond only to memory allocated within the IDABBDPRE module (the banded matrix approximation, banded SUNLINSOL object, temporary vectors). These values are local to each process.

The workspaces referred to here exist in addition to those given by the corresponding function IDAGetLinWorkSpace.

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

IDALS_SUCCESS The optional output value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer was NULL.

IDALS_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 §4.5.10.2), and npsolves and nrevalsLS are linear solver optional outputs (see §4.5.10.5).

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, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapter 7, 8, 9, and 10 for the specific name of the function to be called or macro to be referenced.

Differences between the user main program in §4.4 and the one below start only at step (16). 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, if appropriate**
2. **Set problem dimensions etc.**
3. **Set vectors of initial values**
4. **Create IDAS object**
5. **Initialize IDAS solver**

6. Specify integration tolerances
7. Create matrix object
8. Create linear solver object
9. Set linear solver optional inputs
10. Attach linear solver module
11. Set optional inputs
12. Create nonlinear solver object
13. Attach nonlinear solver module
14. Set nonlinear solver optional inputs
15. Initialize quadrature problem, if not sensitivity-dependent
16. **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]` ($0 \leq$ `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., $\text{plist}_i = i \quad (i = 0, \ldots, N_s - 1)$.

  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.

17. **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.

18. **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).

19. **Set sensitivity tolerances**

    Call `IDASensSStolerances`, `IDASensSVtolerances`, or `IDASensEEtolerances`. See §5.2.2.

20. **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 §5.2.7.

21. **Create sensitivity nonlinear solver object** (*optional*)

    If using a non-default nonlinear solver (see §5.2.3), then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular SUNNONLINSOL implementation e.g.,

    ```
    NLSSens = SUNNonlinSol_***Sens(...);
    ```

    where `***` is the name of the nonlinear solver and `...` are constructor specific arguments (see Chapter 10 for details).

22. **Attach the sensitvity nonlinear solver module** (*optional*)

    If using a non-default nonlinear solver, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling

    ```
    ier = IDASetNonlinearSolverSensSim(ida_mem, NLSSens);
    ```

    when using the `IDA_SIMULTANEOUS` corrector method or

    ```
    ier = IDASetNonlinearSolverSensStg(ida_mem, NLSSens);
    ```

    when using the `IDA_STAGGERED` corrector method (see §5.2.3 for details).

23. **Set sensitivity nonlinear solver optional inputs** (*optional*)

    Call the appropriate set functions for the selected nonlinear solver module to change optional inputs specific to that nonlinear solver. These *must* be called after `IDASensInit` if using the default nonlinear solver or after attaching a new nonlinear solver to IDAS, otherwise the optional inputs will be overridden by IDAS defaults. See Chapter 10 for more information on optional inputs.

24. **Correct initial values**

25. **Specify rootfinding problem**

26. **Advance solution in time**

27. **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 §5.2.6).

28. **Get optional outputs**

29. **Deallocate memory for solution vector**

30. **Deallocate memory for sensitivity vectors**

    Upon completion of the integration, deallocate memory for the vectors contained in `yS0` and `ypS0`:

    ```
    N_VDestroyVectorArray_***(yS0, Ns);
    ```

    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`.

31. **Free user data structure**

32. **Free solver memory**

33. **Free nonlinear solver memory**

34. **Free vector specification memory**

35. **Free linear solver and matrix memory**

36. **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 the default Newton nonlinear solver is used, 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 nonlinear solver interface functions

As in the pure DAE case, when computing solution sensitivities using forward sensitivitiy analysis IDAS uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §10.2) by default. To specify a different nonlinear solver in IDAS, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to IDAS by calling either `IDASetNonlinearSolverSensSim` when using the `IDA_SIMULTANEOUS` corrector option, or `IDASetNonlinearSolver` (see §4.5.4) and `IDASetNonlinearSolverSensStg` when using the `IDA_STAGGERED` corrector option, as documented below.

When changing the nonlinear solver in IDAS, `IDASetNonlinearSolver` must be called after `IDAInit`; similarly `IDASetNonlinearSolverSensSim` and `IDASetNonlinearSolverStg` must be called after `IDASensInit`. If any calls to `IDASolve` have been made, then IDAS will need to be reinitialized by calling `IDAReInit` to ensure that the nonlinear solver is initialized correctly before any subsequent calls to `IDASolve`.

The first argument passed to the routines `IDASetNonlinearSolverSensSim` and `IDASetNonlinearSolverSensStg` is the IDAS memory pointer returned by `IDACreate` and the second argument is the SUNNONLINSOL object to use for solving the nonlinear system 2.4. A call to this function attaches the nonlinear solver to the main IDAS integrator. We note that at present, the SUNNONLINSOL object *must be of type* `SUNNONLINEARSOLVER_ROOTFIND`.

`IDASetNonlinearSolverSensSim`

Call `flag = IDASetNonlinearSolverSensSim(ida_mem, NLS);`

Description The function `IDASetNonLinearSolverSensSim` attaches a SUNNONLINSOL object (`NLS`) to IDAS when using the `IDA_SIMULTANEOUS` approach to correct the state and sensitivity variables at the same time.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `NLS` (`SUNNonlinearSolver`) SUNNONLINSOL object to use for solving nonlinear systems.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The nonlinear solver was successfully attached.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
- `IDA_ILL_INPUT` The SUNNONLINSOL object is `NULL`, does not implement the required nonlinear solver operations, is not of the correct type, or the residual function, convergence test function, or maximum number of nonlinear iterations could not be set.

`IDASetNonlinearSolverSensStg`

Call `flag = IDASetNonlinearSolverSensStg(ida_mem, NLS);`

Description The function `IDASetNonLinearSolverSensStg` attaches a SUNNONLINSOL object (`NLS`) to IDAS when using the `IDA_STAGGERED` approach to correct the sensitivity variables after the correction of the state variables.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block.
- `NLS` (`SUNNonlinearSolver`) SUNNONLINSOL object to use for solving nonlinear systems.

Return value The return value `flag` (of type `int`) is one of
- `IDA_SUCCESS` The nonlinear solver was successfully attached.
- `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.

IDA_ILL_INPUT The SUNNONLINSOL object is NULL, does not implement the required nonlinear solver operations, is not of the correct type, or the residual function, convergence test function, or maximum number of nonlinear iterations could not be set.

Notes This function only attaches the SUNNONLINSOL object for correcting the sensitivity variables. To attach a SUNNONLINSOL object for the state variable correction use IDASetNonlinearSolver (see §4.5.4).

5.2.4 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 §4.5.5.

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 §4.5.5 for a list of possible return values.

5.2.5 IDAS solver function

Even if forward sensitivity analysis was enabled, the call to the main solver function IDASolve is exactly the same as in §4.5.7. 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.

5.2.6 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.

5.2.7 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).

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`	`SUNFALSE`
Maximum no. of nonlinear iterations	`IDASetSensMaxNonlinIters`	3

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`.

`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 (`SUNTRUE`) or not (`SUNFALSE`) 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 `SUNFALSE`. If `errconS`=`SUNTRUE` then both state variables and sensitivity variables are included in the error tests. If `errconS`=`SUNFALSE` 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`.
`IDA_MEM_FAIL` The `ida_mem` SUNNONLINSOL module is `NULL`.

Notes The default value is 3.

5.2.8 Optional outputs for forward sensitivity analysis

5.2.8.1 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.

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`

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.

`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 §5.2.7). 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 a nonlinear solver requiring linear solves 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.
`IDA_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

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.
`IDA_MEM_FAIL`	The SUNNONLINSOL module is `NULL`.

5.2.8.2 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

`Ns`	is the number of sensitivities.
`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. **Initialize IDAS solver**
6. **Specify integration tolerances**
7. **Create matrix object**
8. **Create linear solver object**
9. **Set linear solver optional inputs**

10. Attach linear solver module
11. Set optional inputs
12. Create nonlinear solver object
13. Attach nonlinear solver module
14. Set nonlinear solver optional inputs
15. Initialize sensitivity-independent quadrature problem
16. Define the sensitivity problem
17. Set sensitivity initial conditions
18. Activate sensitivity calculations
19. Set sensitivity tolerances
20. Set sensitivity analysis optional inputs
21. Create sensitivity nonlinear solver object
22. Attach the sensitvity nonlinear solver module
23. Set sensitivity nonlinear solver optional inputs
24. **Set vector of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.
25. **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.
26. **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.
27. Advance solution in time
28. **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.
29. Get optional outputs
30. Extract sensitivity solution
31. **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.
32. Deallocate memory for solutions vector
33. Deallocate memory for sensitivity vectors

34. **Deallocate memory for sensitivity-dependent quadrature variables**

35. **Free solver memory**

36. **Free nonlinear solver memory**

37. **Free vector specification memory**

38. **Free linear solver and matrix memory**

39. **Finalize MPI, if used**

Note: `IDAQuadSensInit` (step 25 above) can be called and quadrature-related optional inputs (step 26 above) can be set, anywhere between steps 16 and 27.

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 §4.5.7. 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 (`SUNTRUE`) or not (`SUNFALSE`) 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 SUNFALSE.

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=SUNTRUE`), `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_Vectors` 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 §7.2 and §7.3).

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, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapters 7, 8, 9, and 10 for the specific name of the function to be called or macro to be referenced.

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 a nonlinear solver requiring a linear solver (e.g., the default Newton iteration) will be used, the 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. **Initialize IDAS solver for the forward problem**
7. **Specify integration tolerances for forward problem**
8. **Set optional inputs for the forward problem**
9. **Create matrix object for the forward problem**
10. **Create linear solver object for the forward problem**
11. **Set linear solver optional inputs for the forward problem**
12. **Attach linear solver module for the forward problem**
13. **Create nonlinear solver module for the forward problem**
14. **Attach nonlinear solver module for the forward problem**
15. **Set nonlinear solver optional inputs for the forward problem**
16. **Initialize quadrature problem or problems for forward problems, using `IDAQuadInit` and/or `IDAQuadSensInit`.**
17. **Initialize forward sensitivity problem**
18. **Specify rootfinding**
19. **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).

20. **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)

21. **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`.

22. **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.

23. **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.

24. **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).

25. **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.

26. **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).

27. **Create matrix object for the backward problem**

    If a nonlinear solver requiring a linear solve will be used (e.g., the the default Newton iteration) and the linear solver will be a direct linear solver, then a template Jacobian matrix must be created by calling the appropriate constructor function defined by the particular SUNMATRIX implementation.

    NOTE: The dense, banded, and sparse matrix objects are usable only in a serial or threaded environment.

    Note also that it is not required to use the same matrix type for both the forward and the backward problems.

28. **Create linear solver object for the backward problem**

    If a nonlinear solver requiring a linear solver is chosen (e.g., the default Newton iteration), then the desired linear solver object for the backward problem must be created by calling the appropriate constructor function defined by the particular SUNLINSOL implementation.

    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 SUNLINSOL_DENSE linear solver module and the backward problem with SUNLINSOL_SPGMR linear solver module.

29. **Set linear solver interface optional inputs for the backward problem**

    Call `IDASet*B` functions to change optional inputs specific to the linear solver interface. See §6.2.9 for details.

30. **Attach linear solver module for the backward problem**

    If a nonlinear solver requiring a linear solver is chosen for the backward problem (e.g., the default Newton iteration), then initialize the IDALS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with the following call (for details see §4.5.3):

    ```
    ier = IDASetLinearSolverB(...);
    ```

31. **Create nonlinear solver object for the backward problem** (*optional*)

    If using a non-default nonlinear solver for the backward problem, then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular SUNNONLINSOL implementation e.g., `NLSB = SUNNonlinSol_***(...);` where `***` is the name of the nonlinear solver (see Chapter 10 for details).

32. **Attach nonlinear solver module for the backward problem** (*optional*)

If using a non-default nonlinear solver for the backward problem, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling
`ier = IDASetNonlinearSolverB(idaode_mem, NLSB);` (see §4.5.4 for details).

33. **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.

34. **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.

35. **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.

36. **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`.

37. **Free the nonlinear solver memory for the forward and backward problems**

38. **Free linear solver and matrix memory for the forward and backward problems**

39. **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 (21)-(35) 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 (21)-(35) 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 §4.5.7) 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 §4.5.7.

`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 §4.5.11 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 are available for the backward problem. They should be created as for the forward problem then attached to the memory structure for the backward problem using the following function.

`IDASetLinearSolverB`

Call `flag = IDASetLinearSolverB(ida_mem, which, LS, A);`

Description The function `IDASetLinearSolverB` attaches a generic SUNLINSOL object `LS` and corresponding template Jacobian SUNMATRIX object `A` (if applicable) to IDAS, initializing the IDALS linear solver interface for solution of the backward problem.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`which` (`int`) represents the identifier of the backward problem returned by `IDACreateB`.

LS (SUNLinearSolver) SUNLINSOL object to use for solving linear systems for the backward problem.

A (SUNMatrix) SUNMATRIX object for used as a template for the Jacobian for the backward problem (or NULL if not applicable).

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

IDALS_SUCCESS The IDALS initialization was successful.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_ILL_INPUT The IDALS interface is not compatible with the LS or A input objects or is incompatible with the current NVECTOR module.

IDALS_MEM_FAIL A memory allocation request failed.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes If LS is a matrix-based linear solver, then the template Jacobian matrix A will be used in the solve process, so if additional storage is required within the SUNMATRIX object (e.g. for factorization of a banded matrix), ensure that the input object is allocated with sufficient size (see the documentation of the particular SUNMATRIX type in Chapter 8 for further information).

The previous routines IDADlsSetLinearSolverB and IDASpilsSetLinearSolverB are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

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 §4.5.5): 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 §4.5.5). 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 §4.5.5). 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 §4.5.7.

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 §4.5.8.1. 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 = IDASetNonlinearSolverB(ida_mem, which, NLSB);
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 Linear solver interface optional input functions

When using matrix-based linear solver modules for the backward problem, i.e., a non-`NULL` SUNMATRIX object `A` was passed to `IDASetLinearSolverB`, the IDALS linear solver interface needs a function to compute an approximation to the Jacobian matrix. This can be attached through a call to either `IDASetJacFnB` or IDAIDASetJacFnBS, with the second used when the backward problem depends on the forward sensitivities.

`IDASetJacFnB`

Call `flag = IDASetJacFnB(ida_mem, which, jacB);`

Description The function `IDASetJacFnB` specifies the Jacobian approximation function to be used for the backward problem.

Arguments `ida_mem` (`void *`) pointer to the IDAS memory block.
`which` (`int`) represents the identifier of the backward problem.
`jacB` (`IDALsJacFnB`) user-defined Jacobian approximation function.

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

`IDALS_SUCCESS` `IDASetJacFnB` succeeded.

IDALS_MEM_NULL The ida_mem was NULL.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_LMEM_NULL The linear solver has not been initialized with a call to IDASetLinearSolverB.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The function type IDALsJacFnB is described in §6.3.5.

The previous routine IDADlsSetJacFnB is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDASetJacFnBS

Call `flag = IDASetJacFnBS(ida_mem, which, jacBS);`

Description The function IDASetJacFnBS specifies the 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 block.

which (int) represents the identifier of the backward problem.

jacBS (IDALJacFnBS) user-defined Jacobian approximation function.

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

IDALS_SUCCESS IDASetJacFnBS succeeded.

IDALS_MEM_NULL The ida_mem was NULL.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_LMEM_NULL The linear solver has not been initialized with a call to IDASetLinearSolverBS.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The function type IDALsJacFnBS is described in §6.3.5.

The previous routine IDADlsSetJacFnBS is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

When using a matrix-free linear solver module for the backward problem, the IDALS linear solver interface requires a function to compute an approximation to the product between the Jacobian matrix $J(t, y)$ and a vector v. This may be performed internally using a difference-quotient approximation, or it may be supplied by the user by calling one of the following two functions:

IDASetJacTimesB

Call `flag = IDASetJacTimesB(ida_mem, which, jsetupB, jtimesB);`

Description The function IDASetJacTimesB specifies the Jacobian-vector setup and product functions to be used.

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

which (int) the identifier of the backward problem.

jtsetupB (IDALsJacTimesSetupFnB) user-defined function to set up the Jacobian-vector product. Pass NULL if no setup is necessary.

jtimesB (IDALsJacTimesVecFnB) user-defined Jacobian-vector product function.

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

IDALS_SUCCESS The optional value has been successfully set.

IDALS_MEM_NULL The ida_mem memory block pointer was NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The function types IDALsJacTimesVecFnB and IDALsJacTimesSetupFnB are described in §6.3.6.

The previous routine IDASpilsSetJacTimesB is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDASetJacTimesBS

Call `flag = IDASetJacTimesBS(ida_mem, which, jsetupBS, jtimesBS);`

Description The function IDASetJacTimesBS specifies the Jacobian-vector product setup and evaluation functions 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.

jtsetupBS (IDALsJacTimesSetupFnBS) user-defined function to set up the Jacobian-vector product. Pass NULL if no setup is necessary.

jtimesBS (IDALsJacTimesVecFnBS) user-defined Jacobian-vector product function.

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

IDALS_SUCCESS The optional value has been successfully set.

IDALS_MEM_NULL The ida_mem memory block pointer was NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The function types IDALsJacTimesVecFnBS and IDALsJacTimesSetupFnBS are described in §6.3.6.

The previous routine IDASpilsSetJacTimesBS is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

Alternately, when using the default difference-quotient approximation to the Jacobian-vector product for the backward problem, the user may specify the factor to use in setting increments for the finite-difference approximation, via a call to IDASetIncrementFactorB:

IDASetIncrementFactorB

Call `flag = IDASetIncrementFactorB(ida_mem, which, dqincfacB);`

Description The function IDASetIncrementFactorB specifies the factor in the increments used in the difference quotient approximations to matrix-vector products for the backward problem.

This routine can be used in both the cases wherethe backward problem does and does not depend on the forward sensitvities.

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

which (int) the identifier of the backward problem.

dqincfacB (realtype) difference quotient approximation factor.

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

IDALS_SUCCESS The optional value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_LMEM_NULL	The IDALS linear solver has not been initialized.
IDALS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDALS_ILL_INPUT	The value of eplifacB is negative.
IDALS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The default value is 1.0.

The previous routine IDASpilsSetIncrementFactorB is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

When using an iterative linear solver for the backward problem, the user may supply a preconditioning operator to aid in solution of the system, or she/he may adjust the convergence tolerance factor for the iterative linear solver. These may be accomplished through calling the following functions:

IDASetPreconditionerB

Call `flag = IDASetPreconditionerB(ida_mem, which, psetupB, psolveB);`

Description The function IDASetPrecSolveFnB 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	(IDALsPrecSetupFnB) user-defined preconditioner setup function.
psolveB	(IDALsPrecSolveFnB) user-defined preconditioner solve function.

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

IDALS_SUCCESS	The optional value has been successfully set.
IDALS_MEM_NULL	The ida_mem memory block pointer was NULL.
IDALS_LMEM_NULL	The IDALS linear solver has not been initialized.
IDALS_NO_ADJ	The function IDAAdjInit has not been previously called.
IDALS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function types IDALsPrecSolveFnB and IDALsPrecSetupFnB are described in §6.3.8 and §6.3.9, respectively. The psetupB argument may be NULL if no setup operation is involved in the preconditioner.

The previous routine IDASpilsSetPreconditionerB is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDASetPreconditionerBS

Call `flag = IDASetPreconditionerBS(ida_mem, which, psetupBS, psolveBS);`

Description The function IDASetPrecSolveFnBS 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	(IDALsPrecSetupFnBS) user-defined preconditioner setup function.
psolveBS	(IDALsPrecSolveFnBS) user-defined preconditioner solve function.

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

IDALS_SUCCESS	The optional value has been successfully set.
IDALS_MEM_NULL	The ida_mem memory block pointer was NULL.
IDALS_LMEM_NULL	The IDALS linear solver has not been initialized.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The function types IDALsPrecSolveFnBS and IDALsPrecSetupFnBS are described in §6.3.8 and §6.3.9, respectively. The psetupBS argument may be NULL if no setup operation is involved in the preconditioner.

The previous routine IDASpilsSetPreconditionerBS is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

IDASetEpsLinB

Call `flag = IDASetEpsLinB(ida_mem, which, eplifacB);`

Description The function IDASetEpsLinB specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the nonlinear iteration test constant. (See §2.1). This routine can be used in both the cases wherethe backward problem does and does not depend on the forward sensitvities.

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

which (int) the identifier of the backward problem.

eplifacB (realtype) linear convergence safety factor (>= 0.0).

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

IDALS_SUCCESS The optional value has been successfully set.

IDALS_MEM_NULL The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_NO_ADJ The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT The value of eplifacB is negative.

IDALS_ILL_INPUT The parameter which represented an invalid identifier.

Notes The default value is 0.05.

Passing a value eplifacB= 0.0 also indicates using the default value.

The previous routine IDASpilsSetEpsLinB is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

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 §4.5.10, 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`.

`IDAGetAdjCheckPointsInfo`

Call `flag = IDAGetAdjCheckPointsInfo(ida_mem, IDAadjCheckPointRec *ckpnt);`

Description The function `IDAGetAdjCheckPointsInfo` loads an array of `ncheck+1` records of type `IDAadjCheckPointRec`. The user must allocate space for the array `ckpnt`.

Arguments
- `ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
- `ckpnt` (`IDAadjCheckPointRec *`) array of `ncheck+1` checkpoint records, each of type `IDAadjCheckPointRec`.

Return value The return value is `IDA_SUCCESS` if successful, or `IDA_MEM_NULL` if `ida_mem` is `NULL`, or `IDA_NO_ADJ` if ASA was not initialized.

Notes The members of each record `ckpnt[i]` are:

- `ckpnt[i].my_addr` (`void *`) address of current checkpoint in `ida_mem->ida_adj_mem`
- `ckpnt[i].next_addr` (`void *`) address of next checkpoint
- `ckpnt[i].t0` (`realtype`) start of checkpoint interval
- `ckpnt[i].t1` (`realtype`) end of checkpoint interval
- `ckpnt[i].nstep` (`long int`) step counter at ckeckpoint `t0`
- `ckpnt[i].order` (`int`) method order at checkpoint `t0`
- `ckpnt[i].step` (`realtype`) step size at checkpoint `t0`

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 applicable for the choice of SUNLINSOL object) 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 §7.2 and §7.3).

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 §7.2 and §7.3).

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 §7.2 and §7.3).

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 §7.2 and §7.3).

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 construction for the backward problem (matrix-based linear solvers)

If a matrix-based linear solver module is is used for the backward problem (i.e., `IDASetLinearSolverB` is called with non-`NULL` SUNMATRIX argument in the step described in §6.1), the user may provide a function of type `IDALsJacFnB` or `IDALsJacFnBS` (see §6.2.9), defined as follows:

`IDALsJacFnB`

Definition
```
typedef int (*IDALsJacFnB)(realtype tt, realtype cjB,
                           N_Vector yy, N_Vector yp,
                           N_Vector yB, N_Vector ypB,
                           N_Vector resvalB,
                           SUNMatrix JacB, void *user_dataB,
                           N_Vector tmp1B, N_Vector tmp2B,
                           N_Vector tmp3B);
```

Purpose This function computes the 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.
`resvalB`	is the current value of the residual for the backward problem.
`JacB`	is the output approximate 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 the `IDALsJacFnB` function as temporary storage or work space.

Return value An `IDALsJacFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDALS sets `last_flag` to `IDALS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `IDASolveB` returns `IDA_LSETUP_FAIL` and IDALS sets `last_flag` to `IDALS_JACFUNC_UNRECVR`).

Notes A user-supplied Jacobian function must load the 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. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 8 for details). Only nonzero elements need to be loaded into `JacB` as this matrix is set to zero before the call to the Jacobian function.

Before calling the user's `IDALsJacFnB`, 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 IDALS sets `last_flag` to `IDALS_JACFUNC_UNRECVR`).

The previous function type IDADlsJacFnB is identical to IDALsJacFnB, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

IDALsJacFnBS

Definition
```
typedef int (*IDALsJacFnBS)(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,
                            SUNMatrix JacB, void *user_dataB,
                            N_Vector tmp1B, N_Vector tmp2B,
                            N_Vector tmp3B);
```

Purpose This function computes the 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.
resvalB	is the current value of the residual for the backward problem.
JacB	is the output approximate 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 IDALsJacFnBS as temporary storage or work space.

Return value An IDALsJacFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDALS sets last_flag to IDALS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, IDASolveB returns IDA_LSETUP_FAIL and IDALS sets last_flag to IDALS_JACFUNC_UNRECVR).

Notes A user-supplied dense Jacobian function must load the 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. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 8 for details). Only nonzero elements need to be loaded into JacB as this matrix is set to zero before the call to the Jacobian function.

Before calling the user's IDALsJacFnBS, 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 IDALS sets last_flag to IDALS_JACFUNC_UNRECVR).

The previous function type IDADlsJacFnBS is identical to IDALsJacFnBS, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

6.3.6 Jacobian-vector product for the backward problem (matrix-free linear solvers)

If a matrix-free linear solver is selected for the backward problem (i.e., IDASetLinearSolverB is called with NULL-valued SUNMATRIX argument in the steps described in §6.1), the user may provide a function of type
IDALsJacTimesVecFnB or IDALsJacTimesVecFnBS in the following form, to compute matrix-vector products Jv. If such a function is not supplied, the default is a difference quotient approximation to these products.

IDALsJacTimesVecFnB

Definition
```
typedef int (*IDALsJacTimesVecFnB)(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 IDALsJacTimesVecFnB as temporary storage or work space.

Return value The return value of a function of type IDALsJtimesVecFnB 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 IDALsJacTimesVecFn (see §4.6.6). If the backward problem is the adjoint of $\dot{y} = f(t, y)$, then this function is to compute $-(\partial f/\partial y)^T v_B$.

The previous function type IDASpilsJacTimesVecFnB is identical to IDALsJacTimesVecFnB, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

IDALsJacTimesVecFnBS

Definition
```
typedef int (*IDALsJacTimesVecFnBS)(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 IDALsJacTimesVecFnBS as temporary storage or work space.

Return value The return value of a function of type IDALsJtimesVecFnBS 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 IDALsJacTimesVecFn (see §4.6.6).

The previous function type IDASpilsJacTimesVecFnBS is identical to IDALsJacTimesVecFnBS, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

6.3.7 Jacobian-vector product setup for the backward problem (matrix-free linear solvers)

If the user's Jacobian-times-vector requires that any Jacobian-related data be preprocessed or evaluated, then this needs to be done in a user-supplied function of type `IDALsJacTimesSetupFnB` or `IDALsJacTimesSetupFnBS`, defined as follows:

`IDALsJacTimesSetupFnB`

Definition
```
typedef int (*IDALsJacTimesSetupFnB)(realtype tt,
                                     N_Vector yy, N_Vector yp,
                                     N_Vector yB, N_Vector ypB,
                                     N_Vector resvalB,
                                     realtype cjB, void *user_dataB);
```

Purpose This function preprocesses and/or evaluates Jacobian data needed by the Jacobian-times-vector routine for the backward problem.

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 $\dot{y}(t)$.
- `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 `IDASetUserDataB`.

Return value The value returned by the Jacobian-vector setup function 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).

Notes Each call to the Jacobian-vector setup function is preceded by a call to the backward problem residual user function with the same `(t,y, yp, yB, ypB)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual.

If the user's `IDALsJacTimesVecFnB` 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_dataB` and then use the `IDAGet*` functions described in §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `IDASpilsJacTimesSetupFnB` is identical to `IDALsJacTimesSetupFnB`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

`IDALsJacTimesSetupFnBS`

Definition
```
typedef int (*IDALsJacTimesSetupFnBS)(realtype tt,
                                      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);
```

Purpose This function preprocesses and/or evaluates Jacobian data needed by the Jacobian-times-vector routine for the backward problem, in the case that the backward problem depends on the forward sensitivities.

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 $\dot{y}(t)$.
- `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 `IDASetUserDataB`.

Return value The value returned by the Jacobian-vector setup function 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).

Notes Each call to the Jacobian-vector setup function is preceded by a call to the backward problem residual user function with the same `(t,y, yp, yyS, ypS, yB, ypB)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual.

If the user's `IDALsJacTimesVecFnB` 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_dataB` and then use the `IDAGet*` functions described in §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `IDASpilsJacTimesSetupFnBS` is identical to `IDALsJacTimesSetupFnBS`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

6.3.8 Preconditioner solve for the backward problem (iterative linear solvers)

If preconditioning is used during integration of the backward problem, then the user must provide a 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:

`IDALsPrecSolveFnB`

Definition
```
typedef int (*IDALsPrecSolveFnB)(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);
```

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.
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).	
Notes	The previous function type IDASpilsPrecSolveFnB is identical to IDALsPrecSolveFnB, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.	

IDALsPrecSolveFnBS

Definition
```
typedef int (*IDALsPrecSolveFnBS)(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);
```

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`.

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).

Notes The previous function type `IDASpilsPrecSolveFnBS` is identical to `IDALsPrecSolveFnBS`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

6.3.9 Preconditioner setup for the backward problem (iterative linear solvers)

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 function of one of the following two types:

`IDALsPrecSetupFnB`

Definition
```
typedef int (*IDALsPrecSetupFnB)(realtype t,
                                 N_Vector yy, N_Vector yp,
                                 N_Vector yB, N_Vector ypB,
                                 N_Vector resvalB,
                                 realtype cjB, void *user_dataB);
```

Purpose This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner for the backward problem.

Arguments The arguments of an `IDALsPrecSetupFnB` 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`.

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).

Notes The previous function type `IDASpilsPrecSetupFnB` is identical to `IDALsPrecSetupFnB`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

`IDALsPrecSetupFnBS`

Definition
```
typedef int (*IDALsPrecSetupFnBS)(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);
```

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 `IDALsPrecSetupFnBS` 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`.

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).

Notes The previous function type `IDASpilsPrecSetupFnBS` is identical to `IDALsPrecSetupFnBS`, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

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* an iterative linear solver for the backward problem has been attached to IDAS by calling `IDASetLinearSolverB` (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:
- `IDALS_SUCCESS` The call to `IDABBDPrecInitB` was successful.
- `IDALS_MEM_FAIL` A memory allocation request has failed.
- `IDALS_MEM_NULL` The `ida_mem` argument was `NULL`.
- `IDALS_LMEM_NULL` No linear solver has been attached.
- `IDALS_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:
- `IDALS_SUCCESS` The call to `IDABBDPrecReInitB` was successful.
- `IDALS_MEM_FAIL` A memory allocation request has failed.
- `IDALS_MEM_NULL` The `ida_mem` argument was `NULL`.
- `IDALS_PMEM_NULL` The `IDABBDPrecInitB` has not been previously called.
- `IDALS_LMEM_NULL` No linear solver has been attached.
- `IDALS_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 the implementations provided with SUNDIALS. The generic operations are described below and the implementations provided with SUNDIALS are described in the following sections.

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);
  int          (*nvlinearcombination)(int, realtype*, N_Vector*, N_Vector);
  int          (*nvscaleaddmulti)(int, realtype*, N_Vector, N_Vector*, N_Vector*);
  int          (*nvdotprodmulti)(int, N_Vector, N_Vector*, realtype*);
  int          (*nvlinearsumvectorarray)(int, realtype, N_Vector*, realtype,
                                         N_Vector*, N_Vector*);
  int          (*nvscalevectorarray)(int, realtype*, N_Vector*, N_Vector*);
  int          (*nvconstvectorarray)(int, realtype, N_Vector*);
  int          (*nvwrmsnomrvectorarray)(int, N_Vector*, N_Vector*, realtype*);
  int          (*nvwrmsnomrmaskvectorarray)(int, N_Vector*, N_Vector, N_Vector,
                                            realtype*);
  int          (*nvscaleaddmultivectorarray)(int, int, realtype*, N_Vector*,
                                             N_Vector**, N_Vector**);
  int          (*nvlinearcombinationvectorarray)(int, int, realtype*, N_Vector**,
                                                 N_Vector*);
};
```

The generic NVECTOR module defines and implements the vector operations acting on an `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 standard vector operations defined by the generic NVECTOR module. Tables 7.3 and 7.4 list *optional* fused and vector array operations respectively.

Fused and vector array operations are intended to increase data reuse, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. If a particular NVECTOR implementation defines a fused or vector array operation as `NULL`, the generic NVECTOR module will automatically call standard vector operations as necessary to complete the desired operation. Currently, all fused and vector array operations are disabled by default however, SUNDIALS provided NVECTOR implementations define additional user-callable functions to enable/disable any or all of the fused and vector array operations. See the following sections for the implementation specific functions to enable/disable operations.

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

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_OPENMPDEV	OpenMP shared memory parallel with device offloading	6
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	7

```
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 7.2: 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.
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.

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Name	Usage and Description
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`: $y_i = \lvert x_i \rvert$, $i = 0, \ldots, n-1$.
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`: $m = \max_i \lvert x_i \rvert$.

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Name	Usage and Description
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 positive elements of the `N_Vector id`: $m = \sqrt{\left(\sum_{i=0}^{n-1}(x_i w_i H(id_i))^2\right)/n}$, where $H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$
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.
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 `SUNTRUE` if all components of `x` are nonzero (successful inversion) and returns `SUNFALSE` 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 `SUNFALSE` if any element failed the constraint test and assigned to `SUNTRUE` 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.

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Name	Usage and Description
N_VMinQuotient	`minq = N_VMinQuotient(num, denom);` This routine returns the minimum of the quotients obtained by term-wise 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.

Table 7.3: Description of the NVECTOR fused operations

Name	Usage and Description
N_VLinearCombination	`ier = N_VLinearCombination(nv, c, X, z);` This routine computes the linear combination of n_v vectors with n elements: $$z_i = \sum_{j=0}^{n_v-1} c_j x_{j,i}, \quad i = 0, \ldots, n-1,$$ where c is an array of n_v scalars (type `realtype`*), X is an array of n_v vectors (type `N_Vector*`), and z is the output vector (type `N_Vector`). If the output vector z is one of the vectors in X, then it *must* be the first vector in the vector array. The operation returns `0` for success and a non-zero value otherwise.
N_VScaleAddMulti	`ier = N_VScaleAddMulti(nv, c, x, Y, Z);` This routine scales and adds one vector to n_v vectors with n elements: $$z_{j,i} = c_j x_i + y_{j,i}, \quad j = 0, \ldots, n_v - 1 \quad i = 0, \ldots, n-1,$$ where c is an array of n_v scalars (type `realtype`*), x is the vector (type `N_Vector`) to be scaled and added to each vector in the vector array of n_v vectors Y (type `N_Vector*`), and Z (type `N_Vector*`) is a vector array of n_v output vectors. The operation returns `0` for success and a non-zero value otherwise.

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Name	Usage and Description
N_VDotProdMulti	`ier = N_VDotProdMulti(nv, x, Y, d);` This routine computes the dot product of a vector with n_v other vectors: $$d_j = \sum_{i=0}^{n-1} x_i y_{j,i}, \quad j = 0, \ldots, n_v - 1,$$ where d (type `realtype`*) is an array of n_v scalars containing the dot products of the vector x (type `N_Vector`) with each of the n_v vectors in the vector array Y (type `N_Vector*`). The operation returns `0` for success and a non-zero value otherwise.

Table 7.4: Description of the NVECTOR vector array operations

Name	Usage and Description
N_VLinearSumVectorArray	`ier = N_VLinearSumVectorArray(nv, a, X, b, Y, Z);` This routine comuptes the linear sum of two vector arrays containing n_v vectors of n elements: $$z_{j,i} = ax_{j,i} + by_{j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$ where a and b are `realtype` scalars and X, Y, and Z are arrays of n_v vectors (type `N_Vector*`). The operation returns `0` for success and a non-zero value otherwise.
N_VScaleVectorArray	`ier = N_VScaleVectorArray(nv, c, X, Z);` This routine scales each vector of n elements in a vector array of n_v vectors by a potentially different constant: $$z_{j,i} = c_j x_{j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$ where c is an array of n_v scalars (type `realtype`*) and X and Z are arrays of n_v vectors (type `N_Vector*`). The operation returns `0` for success and a non-zero value otherwise.

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Name	**Usage and Description**
`N_VConstVectorArray`	`ier = N_VConstVectorArray(nv, c, X);` This routine sets each element in a vector of n elements in a vector array of n_v vectors to the same value: $$z_{j,i} = c, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$ where c is a `realtype` scalar and X is an array of n_v vectors (type `N_Vector*`). The operation returns `0` for success and a non-zero value otherwise.
`N_VWrmsNormVectorArray`	`ier = N_VWrmsNormVectorArray(nv, X, W, m);` This routine computes the weighted root mean square norm of n_v vectors with n elements: $$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i})^2 \right)^{1/2}, \quad j = 0, \ldots, n_v - 1,$$ where m (type `realtype*`) contains the n_v norms of the vectors in the vector array X (type `N_Vector*`) with corresponding weight vectors W (type `N_Vector*`). The operation returns `0` for success and a non-zero value otherwise.
`N_VWrmsNormMaskVectorArray`	`ier = N_VWrmsNormMaskVectorArray(nv, X, W, id, m);` This routine computes the masked weighted root mean square norm of n_v vectors with n elements: $$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i} H(id_i))^2 \right)^{1/2}, \quad j = 0, \ldots, n_v - 1,$$ $H(id_i) = 1$ for $id_i > 0$ and is zero otherwise, m (type `realtype*`) contains the n_v norms of the vectors in the vector array X (type `N_Vector*`) with corresponding weight vectors W (type `N_Vector*`) and mask vector id (type `N_Vector`). The operation returns `0` for success and a non-zero value otherwise.

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Name	Usage and Description
`N_VScaleAddMultiVectorArray`	`ier = N_VScaleAddMultiVectorArray(nv, ns, c, X, YY, ZZ);` This routine scales and adds a vector in a vector array of n_v vectors to the corresponding vector in n_s vector arrays: $$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0,\dots,n-1 \quad j = 0,\dots,n_v-1,$$ where c is an array of n_s scalars (type `realtype*`), X is a vector array of n_v vectors (type idN_Vector*) to be scaled and added to the corresponding vector in each of the n_s vector arrays in the array of vector arrays YY (type `N_Vector**`) and stored in the output array of vector arrays ZZ (type `N_Vector**`). The operation returns `0` for success and a non-zero value otherwise.
`N_VLinearCombinationVectorArray`	`ier = N_VLinearCombinationVectorArray(nv, ns, c, XX, Z);` This routine computes the linear combination of n_s vector arrays containing n_v vectors with n elements: $$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0,\dots,n-1 \quad j = 0,\dots,n_v-1,$$ where c is an array of n_s scalars (type `realtype*`), XX (type `N_Vector**`) is an array of n_s vector arrays each containing n_v vectors to be summed into the output vector array of n_v vectors Z (type `N_Vector*`). If the output vector array Z is one of the vector arrays in XX, then it *must* be the first vector array in XX. The operation returns `0` for success and a non-zero value otherwise.

7.1 NVECTOR functions used by IDAS

In Table 7.5 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 columns show function usage within the IDAS linear solvers interface, the IDABBDPRE preconditioner module, and the IDAA module.

At this point, we should emphasize that the IDAS user does not need to know anything about the usage of vector functions by the IDAS code modules in order to use IDAS. The information is presented as an implementation detail for the interested reader.

Special cases (numbers match markings in table):

1. These routines are only required if an internal difference-quotient routine for constructing dense or band Jacobian matrices is used.

2. This routine is optional, and is only used in estimating space requirements for IDAS modules for user feedback.

3. The optional function `N_VDotProdMulti` is only used when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR. The remaining operations from Tables 7.3 and 7.4 not listed above are

unused and a user-supplied NVECTOR module for IDAS could omit these operations.

Of the functions listed in Table 7.2, N_VWL2Norm, N_VL1Norm, and N_VInvTest are *not* used by IDAS. Therefore a user-supplied NVECTOR module for IDAS could omit these functions.

7.2 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 include when using this module is nvector_serial.h. The installed module library to link to is libsundials_nvecserial.*lib* where *.lib* is typically .so for shared libraries and .a for static libraries.

7.2.1 NVECTOR_SERIAL accessor macros

The following 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] )
  ```

7.2.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4. Their names are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix `_Serial` (e.g. `N_VDestroy_Serial`). All the standard vector operations listed in 7.2 with the suffix `_Serial` appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. `FN_VDestroy_Serial`).

The module NVECTOR_SERIAL provides the following additional user-callable routines:

`N_VNew_Serial`

Prototype `N_Vector N_VNew_Serial(sunindextype vec_length);`

Description This function creates and allocates memory for a serial `N_Vector`. Its only argument is the vector length.

F2003 Name This function is callable as `FN_VNew_Serial` when using the Fortran 2003 interface module.

`N_VNewEmpty_Serial`

Prototype `N_Vector N_VNewEmpty_Serial(sunindextype vec_length);`

Description This function creates a new serial `N_Vector` with an empty (`NULL`) data array.

F2003 Name This function is callable as `FN_VNewEmpty_Serial` when using the Fortran 2003 interface module.

`N_VMake_Serial`

Prototype `N_Vector N_VMake_Serial(sunindextype vec_length, realtype *v_data);`

Description 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.)

F2003 Name This function is callable as `FN_VMake_Serial` when using the Fortran 2003 interface module.

`N_VCloneVectorArray_Serial`

Prototype `N_Vector *N_VCloneVectorArray_Serial(int count, N_Vector w);`

Description This function creates (by cloning) an array of `count` serial vectors.

`N_VCloneVectorArrayEmpty_Serial`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_Serial(int count, N_Vector w);`

Description This function creates (by cloning) an array of `count` serial vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_Serial`

Prototype `void N_VDestroyVectorArray_Serial(N_Vector *vs, int count);`

Description 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`.

`N_VGetLength_Serial`

Prototype `sunindextype N_VGetLength_Serial(N_Vector v);`

Description This function returns the number of vector elements.

F2003 Name This function is callable as `FN_VGetLength_Serial` when using the Fortran 2003 interface module.

`N_VPrint_Serial`

Prototype `void N_VPrint_Serial(N_Vector v);`

Description This function prints the content of a serial vector to `stdout`.

F2003 Name This function is callable as `FN_VPrint_Serial` when using the Fortran 2003 interface module.

`N_VPrintFile_Serial`

Prototype `void N_VPrintFile_Serial(N_Vector v, FILE *outfile);`

Description This function prints the content of a serial vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_SERIAL module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_Serial`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_Serial` will have the default settings for the NVECTOR_SERIAL module.

`N_VEnableFusedOps_Serial`

Prototype `int N_VEnableFusedOps_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Serial`

Prototype `int N_VEnableLinearCombination_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Serial`

Prototype `int N_VEnableScaleAddMulti_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_Serial`

Prototype `int N_VEnableDotProdMulti_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Serial`

Prototype `int N_VEnableLinearSumVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Serial`

Prototype `int N_VEnableScaleVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Serial`

Prototype `int N_VEnableConstVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_Serial`

Prototype `int N_VEnableWrmsNormVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_Serial`

Prototype `int N_VEnableWrmsNormMaskVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_Serial`

Prototype `int N_VEnableScaleAddMultiVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_Serial`

Prototype `int N_VEnableLinearCombinationVectorArray_Serial(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the serial vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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* = `SUNFALSE`. `N_VDestroy_Serial` and `N_VDestroyVectorArray_Serial` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. 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.

7.2.3 NVECTOR_SERIAL Fortran interfaces

The NVECTOR_SERIAL module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fnvector_serial_mod` FORTRAN module defines interfaces to all NVECTOR_SERIAL C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `N_VNew_Serial` is interfaced as `FN_VNew_Serial`.

The FORTRAN 2003 NVECTOR_SERIAL interface module can be accessed with the `use` statement, i.e. `use fnvector_serial_mod`, and linking to the library `libsundials_fnvectorserial_mod.`*lib* in addition to the C library. For details on where the library and module file `fnvector_serial_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fnvectorserial_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 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.

7.3 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 include when using this module is `nvector_parallel.h`. The installed module library to link to is `libsundials_nvecparallel.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

7.3.1 NVECTOR_PARALLEL accessor macros

The following 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] )
  ```

7.3.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4. Their names are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix `_Parallel` (e.g. `N_VDestroy_Parallel`). The module NVECTOR_PARALLEL provides the following additional user-callable routines:

`N_VNew_Parallel`

Prototype
```
N_Vector N_VNew_Parallel(MPI_Comm comm, sunindextype local_length,
                         sunindextype global_length);
```

Description This function creates and allocates memory for a parallel vector.

`N_VNewEmpty_Parallel`

Prototype
```
N_Vector N_VNewEmpty_Parallel(MPI_Comm comm, sunindextype local_length,
                              sunindextype global_length);
```

Description This function creates a new parallel `N_Vector` with an empty (`NULL`) data array.

`N_VMake_Parallel`

Prototype
```
N_Vector N_VMake_Parallel(MPI_Comm comm, sunindextype local_length,
                          sunindextype global_length, realtype *v_data);
```

Description 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_VCloneVectorArray_Parallel`

Prototype
```
N_Vector *N_VCloneVectorArray_Parallel(int count, N_Vector w);
```

Description This function creates (by cloning) an array of `count` parallel vectors.

`N_VCloneVectorArrayEmpty_Parallel`

Prototype
```
N_Vector *N_VCloneVectorArrayEmpty_Parallel(int count, N_Vector w);
```

Description This function creates (by cloning) an array of `count` parallel vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_Parallel`

Prototype
```
void N_VDestroyVectorArray_Parallel(N_Vector *vs, int count);
```

Description 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`.

`N_VGetLength_Parallel`

Prototype
```
sunindextype N_VGetLength_Parallel(N_Vector v);
```

Description This function returns the number of vector elements (global vector length).

`N_VGetLocalLength_Parallel`

Prototype
```
sunindextype N_VGetLocalLength_Parallel(N_Vector v);
```

Description This function returns the local vector length.

`N_VPrint_Parallel`

Prototype `void N_VPrint_Parallel(N_Vector v);`

Description This function prints the local content of a parallel vector to `stdout`.

`N_VPrintFile_Parallel`

Prototype `void N_VPrintFile_Parallel(N_Vector v, FILE *outfile);`

Description This function prints the local content of a parallel vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_PARALLEL module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_Parallel`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone` with that vector. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_Parallel` will have the default settings for the NVECTOR_PARALLEL module.

`N_VEnableFusedOps_Parallel`

Prototype `int N_VEnableFusedOps_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Parallel`

Prototype `int N_VEnableLinearCombination_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Parallel`

Prototype `int N_VEnableScaleAddMulti_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_Parallel`

Prototype `int N_VEnableDotProdMulti_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Parallel`

Prototype `int N_VEnableLinearSumVectorArray_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Parallel`

Prototype `int N_VEnableScaleVectorArray_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Parallel`

Prototype `int N_VEnableConstVectorArray_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_Parallel`

Prototype `int N_VEnableWrmsNormVectorArray_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_Parallel`

Prototype `int N_VEnableWrmsNormMaskVectorArray_Parallel(N_Vector v, booleantype tf);`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_Parallel`

Prototype
```
int N_VEnableScaleAddMultiVectorArray_Parallel(N_Vector v,
                                               booleantype tf);
```

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_Parallel`

Prototype
```
int N_VEnableLinearCombinationVectorArray_Parallel(N_Vector v,
                                                   booleantype tf);
```

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the parallel vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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* = `SUNFALSE`. `N_VDestroy_Parallel` and `N_VDestroyVectorArray_Parallel` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. 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.

7.3.3 NVECTOR_PARALLEL Fortran interfaces

For solvers that include a FORTRAN 77 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.

7.4 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 include when using this module is `nvector_openmp.h`. The installed module library to link to is `libsundials_nvecopenmp.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries. The FORTRAN module file to use when using the FORTRAN 2003 interface to this module is `fnvector_openmp_mod.mod`.

7.4.1 NVECTOR_OPENMP accessor macros

The following 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] )
```

7.4.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4. Their names are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix _OpenMP (e.g. N_VDestroy_OpenMP). All the standard vector operations listed in 7.2 with the suffix _OpenMP appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FN_VDestroy_OpenMP).

The module NVECTOR_OPENMP provides the following additional user-callable routines:

N_VNew_OpenMP

Prototype `N_Vector N_VNew_OpenMP(sunindextype vec_length, int num_threads)`

Description This function creates and allocates memory for a OpenMP N_Vector. Arguments are the vector length and number of threads.

F2003 Name This function is callable as FN_VNew_OpenMP when using the Fortran 2003 interface module.

N_VNewEmpty_OpenMP

Prototype `N_Vector N_VNewEmpty_OpenMP(sunindextype vec_length, int num_threads)`

Description This function creates a new OpenMP N_Vector with an empty (NULL) data array.

F2003 Name This function is callable as FN_VNewEmpty_OpenMP when using the Fortran 2003 interface module.

`N_VMake_OpenMP`

Prototype `N_Vector N_VMake_OpenMP(sunindextype vec_length, realtype *v_data, int num_threads);`

Description 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.

F2003 Name This function is callable as `FN_VMake_OpenMP` when using the Fortran 2003 interface module.

`N_VCloneVectorArray_OpenMP`

Prototype `N_Vector *N_VCloneVectorArray_OpenMP(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` OpenMP vectors.

`N_VCloneVectorArrayEmpty_OpenMP`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_OpenMP(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` OpenMP vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_OpenMP`

Prototype `void N_VDestroyVectorArray_OpenMP(N_Vector *vs, int count)`

Description 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`.

`N_VGetLength_OpenMP`

Prototype `sunindextype N_VGetLength_OpenMP(N_Vector v)`

Description This function returns number of vector elements.

F2003 Name This function is callable as `FN_VGetLength_OpenMP` when using the Fortran 2003 interface module.

`N_VPrint_OpenMP`

Prototype `void N_VPrint_OpenMP(N_Vector v)`

Description This function prints the content of an OpenMP vector to `stdout`.

F2003 Name This function is callable as `FN_VPrint_OpenMP` when using the Fortran 2003 interface module.

`N_VPrintFile_OpenMP`

Prototype `void N_VPrintFile_OpenMP(N_Vector v, FILE *outfile)`

Description This function prints the content of an OpenMP vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_OPENMP module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_OpenMP`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_OpenMP` will have the default settings for the NVECTOR_OPENMP module.

`N_VEnableFusedOps_OpenMP`

Prototype `int N_VEnableFusedOps_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_OpenMP`

Prototype `int N_VEnableLinearCombination_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_OpenMP`

Prototype `int N_VEnableScaleAddMulti_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_OpenMP`

Prototype `int N_VEnableDotProdMulti_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_OpenMP`

Prototype `int N_VEnableLinearSumVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_OpenMP`

Prototype `int N_VEnableScaleVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_OpenMP`

Prototype `int N_VEnableConstVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_OpenMP`

Prototype `int N_VEnableWrmsNormVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_OpenMP`

Prototype `int N_VEnableWrmsNormMaskVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_OpenMP`

Prototype `int N_VEnableScaleAddMultiVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_OpenMP`

Prototype `int N_VEnableLinearCombinationVectorArray_OpenMP(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the OpenMP vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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* = `SUNFALSE`. `N_VDestroy_OpenMP` and `N_VDestroyVectorArray_OpenMP` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. 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.

7.4.3 NVECTOR_OPENMP Fortran interfaces

The NVECTOR_OPENMP module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `nvector_openmp_mod` FORTRAN module defines interfaces to most NVECTOR_OPENMP C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `N_VNew_OpenMP` is interfaced as `FN_VNew_OpenMP`.

The FORTRAN 2003 NVECTOR_OPENMP interface module can be accessed with the `use` statement, i.e. `use fnvector_openmp_mod`, and linking to the library `libsundials_fnvectoropenmp_mod.`*lib* in addition to the C library. For details on where the library and module file `fnvector_openmp_mod.mod` are installed see Appendix A.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 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.

7.5 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 include when using this module is `nvector_pthreads.h`. The installed module library to link to is `libsundials_nvecpthreads.`*lib* where *.lib* is typically `.so` for shared libraries and `.a` for static libraries.

7.5.1 NVECTOR_PTHREADS accessor macros

The following 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] )
```

7.5.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4. Their names are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix _Pthreads (e.g. N_VDestroy_Pthreads). All the standard vector operations listed in 7.2 are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FN_VDestroy_Pthreads). The module NVECTOR_PTHREADS provides the following additional user-callable routines:

N_VNew_Pthreads

Prototype `N_Vector N_VNew_Pthreads(sunindextype vec_length, int num_threads)`

Description This function creates and allocates memory for a Pthreads N_Vector. Arguments are the vector length and number of threads.

F2003 Name This function is callable as FN_VNew_Pthreads when using the Fortran 2003 interface module.

N_VNewEmpty_Pthreads

Prototype `N_Vector N_VNewEmpty_Pthreads(sunindextype vec_length, int num_threads)`

Description This function creates a new Pthreads N_Vector with an empty (NULL) data array.

F2003 Name This function is callable as FN_VNewEmpty_Pthreads when using the Fortran 2003 interface module.

`N_VMake_Pthreads`

Prototype `N_Vector N_VMake_Pthreads(sunindextype vec_length, realtype *v_data, int num_threads);`

Description 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.

F2003 Name This function is callable as `FN_VMake_Pthreads` when using the Fortran 2003 interface module.

`N_VCloneVectorArray_Pthreads`

Prototype `N_Vector *N_VCloneVectorArray_Pthreads(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` Pthreads vectors.

`N_VCloneVectorArrayEmpty_Pthreads`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_Pthreads(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` Pthreads vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_Pthreads`

Prototype `void N_VDestroyVectorArray_Pthreads(N_Vector *vs, int count)`

Description 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`.

`N_VGetLength_Pthreads`

Prototype `sunindextype N_VGetLength_Pthreads(N_Vector v)`

Description This function returns the number of vector elements.

F2003 Name This function is callable as `FN_VGetLength_Pthreads` when using the Fortran 2003 interface module.

`N_VPrint_Pthreads`

Prototype `void N_VPrint_Pthreads(N_Vector v)`

Description This function prints the content of a Pthreads vector to `stdout`.

F2003 Name This function is callable as `FN_VPrint_Pthreads` when using the Fortran 2003 interface module.

`N_VPrintFile_Pthreads`

Prototype `void N_VPrintFile_Pthreads(N_Vector v, FILE *outfile)`

Description This function prints the content of a Pthreads vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_PTHREADS module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_Pthreads`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_Pthreads` will have the default settings for the NVECTOR_PTHREADS module.

`N_VEnableFusedOps_Pthreads`

Prototype `int N_VEnableFusedOps_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Pthreads`

Prototype `int N_VEnableLinearCombination_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Pthreads`

Prototype `int N_VEnableScaleAddMulti_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_Pthreads`

Prototype `int N_VEnableDotProdMulti_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Pthreads`

Prototype `int N_VEnableLinearSumVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Pthreads`

Prototype `int N_VEnableScaleVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Pthreads`

Prototype `int N_VEnableConstVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_Pthreads`

Prototype `int N_VEnableWrmsNormVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_Pthreads`

Prototype `int N_VEnableWrmsNormMaskVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_Pthreads`

Prototype `int N_VEnableScaleAddMultiVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_Pthreads`

Prototype `int N_VEnableLinearCombinationVectorArray_Pthreads(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the Pthreads vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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* = `SUNFALSE`. `N_VDestroy_Pthreads` and `N_VDestroyVectorArray_Pthreads` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. 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.

7.5.3 NVECTOR_PTHREADS Fortran interfaces

The NVECTOR_PTHREADS module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `nvector_pthreads_mod` FORTRAN module defines interfaces to most NVECTOR_PTHREADS C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `N_VNew_Pthreads` is interfaced as `FN_VNew_Pthreads`.

The FORTRAN 2003 NVECTOR_PTHREADS interface module can be accessed with the `use` statement, i.e. `use fnvector_pthreads_mod`, and linking to the library `libsundials_fnvectorpthreads_mod.`*lib* in addition to the C library. For details on where the library and module file `fnvector_pthreads_mod.mod` are installed see Appendix A.

FORTRAN 77 interface functions

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.

7.6 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 include when using this module is `nvector_parhyp.h`. The installed module library to link to is `libsundials_nvecparhyp.`*lib* where *.lib* is typically `.so` for shared libraries and `.a` for static libraries.

Unlike native SUNDIALS vector types, NVECTOR_PARHYP does not provide macros to access its member variables. Note that NVECTOR_PARHYP requires SUNDIALS to be built with MPI support.

7.6.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4, 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 the *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 [31] and the `ark_diurnal_kry_ph.c` example program for ARKODE [39].

The names of parhyp methods are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR_PARHYP provides the following additional user-callable routines:

`N_VNewEmpty_ParHyp`

Prototype `N_Vector N_VNewEmpty_ParHyp(MPI_Comm comm, sunindextype local_length, sunindextype global_length)`

Description This function creates a new parhyp `N_Vector` with the pointer to the *hypre* vector set to `NULL`.

`N_VMake_ParHyp`

Prototype `N_Vector N_VMake_ParHyp(HYPRE_ParVector x)`

Description This function creates an `N_Vector` wrapper around an existing *hypre* parallel vector. It does *not* allocate memory for `x` itself.

`N_VGetVector_ParHyp`

Prototype `HYPRE_ParVector N_VGetVector_ParHyp(N_Vector v)`

Description This function returns the underlying *hypre* vector.

`N_VCloneVectorArray_ParHyp`

Prototype `N_Vector *N_VCloneVectorArray_ParHyp(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` parallel vectors.

`N_VCloneVectorArrayEmpty_ParHyp`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_ParHyp(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` parallel vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_ParHyp`

Prototype `void N_VDestroyVectorArray_ParHyp(N_Vector *vs, int count)`

Description 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`.

`N_VPrint_ParHyp`

Prototype `void N_VPrint_ParHyp(N_Vector v)`

Description This function prints the local content of a parhyp vector to `stdout`.

`N_VPrintFile_ParHyp`

Prototype `void N_VPrintFile_ParHyp(N_Vector v, FILE *outfile)`

Description This function prints the local content of a parhyp vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_PARHYP module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VMake_ParHyp`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VMake_ParHyp` will have the default settings for the NVECTOR_PARHYP module.

`N_VEnableFusedOps_ParHyp`

Prototype `int N_VEnableFusedOps_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_ParHyp`

Prototype `int N_VEnableLinearCombination_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_ParHyp`

Prototype `int N_VEnableScaleAddMulti_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_ParHyp`

Prototype `int N_VEnableDotProdMulti_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_ParHyp`

Prototype `int N_VEnableLinearSumVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_ParHyp`

Prototype `int N_VEnableScaleVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_ParHyp`

Prototype `int N_VEnableConstVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_ParHyp`

Prototype `int N_VEnableWrmsNormVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_ParHyp`

Prototype `int N_VEnableWrmsNormMaskVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_ParHyp`

Prototype `int N_VEnableScaleAddMultiVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_ParHyp`

Prototype `int N_VEnableLinearCombinationVectorArray_ParHyp(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the parhyp vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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 `SUNFALSE`. `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 `SUNFALSE`. 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.

7.7 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 include when using this module is `nvector_petsc.h`. The installed module library to link to is `libsundials_nvecpetsc.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

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.

7.7.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4, 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 [29].

The names of vector operations are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix `_Petsc` (e.g. `N_VDestroy_Petsc`). The module NVECTOR_PETSC provides the following additional user-callable routines:

`N_VNewEmpty_Petsc`

Prototype `N_Vector N_VNewEmpty_Petsc(MPI_Comm comm, sunindextype local_length, sunindextype global_length)`

Description 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_VMake_Petsc`

Prototype `N_Vector N_VMake_Petsc(Vec *pvec)`

Description 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_VGetVector_Petsc`

Prototype `Vec *N_VGetVector_Petsc(N_Vector v)`

Description This function returns a pointer to the underlying PETSc vector.

`N_VCloneVectorArray_Petsc`

Prototype `N_Vector *N_VCloneVectorArray_Petsc(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` NVECTOR_PETSC vectors.

`N_VCloneVectorArrayEmpty_Petsc`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_Petsc(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` NVECTOR_PETSC vectors, each with pointers to PETSc vectors set to (`NULL`).

`N_VDestroyVectorArray_Petsc`

Prototype `void N_VDestroyVectorArray_Petsc(N_Vector *vs, int count)`

Description 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`.

`N_VPrint_Petsc`

Prototype `void N_VPrint_Petsc(N_Vector v)`

Description This function prints the global content of a wrapped PETSc vector to `stdout`.

`N_VPrintFile_Petsc`

Prototype `void N_VPrintFile_Petsc(N_Vector v, const char fname[])`

Description This function prints the global content of a wrapped PETSc vector to `fname`.

By default all fused and vector array operations are disabled in the NVECTOR_PETSC module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VMake_Petsc`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VMake_Petsc` will have the default settings for the NVECTOR_PETSC module.

`N_VEnableFusedOps_Petsc`

Prototype `int N_VEnableFusedOps_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Petsc`

Prototype `int N_VEnableLinearCombination_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Petsc`

Prototype `int N_VEnableScaleAddMulti_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_Petsc`

Prototype `int N_VEnableDotProdMulti_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Petsc`

Prototype `int N_VEnableLinearSumVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Petsc`

Prototype `int N_VEnableScaleVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Petsc`

Prototype `int N_VEnableConstVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_Petsc`

Prototype `int N_VEnableWrmsNormVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_Petsc`

Prototype `int N_VEnableWrmsNormMaskVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_Petsc`

Prototype `int N_VEnableScaleAddMultiVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_Petsc`

Prototype `int N_VEnableLinearCombinationVectorArray_Petsc(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the PETSc vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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 `SUNFALSE`. `N_VDestroy_Petsc` and `N_VDestroyVectorArray_Petsc` will not attempt to free the pointer *pvec* for any `N_Vector` with *own_data* set to `SUNFALSE`. 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.

7.8 The NVECTOR_CUDA implementation

The NVECTOR_CUDA module is an experimental NVECTOR implementation 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 the namespace `suncudavec` manages the vector data layout:

```
template <class T, class I>
class Vector {
  I size_;
  I mem_size_;
  I global_size_;
  T* h_vec_;
  T* d_vec_;
  ThreadPartitioning<T, I>* partStream_;
  ThreadPartitioning<T, I>* partReduce_;
  bool ownPartitioning_;
  bool ownData_;
  bool managed_mem_;
  SUNMPI_Comm comm_;
  ...
};
```

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 `ThreadPartitioning` implementations that handle thread partitioning for streaming and reduction vector kernels, a boolean flag that signals if the vector owns the thread partitioning, a boolean flag that signals if the vector owns the data, a boolean flag that signals if managed memory is used for the data arrays, and the MPI communicator. The class `Vector` inherits from the empty structure

```
struct _N_VectorContent_Cuda {};
```

to interface the C++ class with the NVECTOR C code. 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.

When instantiated with `N_VNew_Cuda`, the class `Vector` will allocate memory on both the host and the device. Alternatively, a user can provide host and device data arrays by using the `N_VMake_Cuda`

constructor. To use CUDA managed memory, the constructors `N_VNewManaged_Cuda` and `N_VMakeManaged_Cuda` are provided. Details on each of these constructors are provided below.

The NVECTOR_CUDA module can be utilized for single-node parallelism or in a distributed context with MPI. In the single-node case the header file to include `nvector_cuda.h` and the library to link to is `libsundials_nveccuda.`*lib*. In the a distributed setting the header file to include is `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda.`*lib*. The extension, *.lib*, is typically `.so` for shared libraries and `.a` for static libraries. Only one of these libraries may be linked to when creating an executable or library. SUNDIALS must be built with MPI support if the distributed library is desired.

7.8.1 NVECTOR_CUDA functions

Unlike other native SUNDIALS vector types, NVECTOR_CUDA does not provide macros to access its member variables. Instead, user should use the accessor functions:

`N_VGetLength_Cuda`

Prototype `sunindextype N_VGetLength_Cuda(N_Vector v)`

Description This function returns the global length of the vector.

`N_VGetLocalLength_Cuda`

Prototype `sunindextype N_VGetLocalLength_Cuda(N_Vector v)`

Description This function returns the local length of the vector.

Note: This function is for use in a *distributed* context and is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

`N_VGetHostArrayPointer_Cuda`

Prototype `realtype *N_VGetHostArrayPointer_Cuda(N_Vector v)`

Description This function returns a pointer to the vector data on the host.

`N_VGetDeviceArrayPointer_Cuda`

Prototype `realtype *N_VGetDeviceArrayPointer_Cuda(N_Vector v)`

Description This function returns a pointer to the vector data on the device.

`N_VGetMPIComm_Cuda`

Prototype `MPI_Comm N_VGetMPIComm_Cuda(N_Vector v)`

Description This function returns the MPI communicator for the vector.

Note: This function is for use in a *distributed* context and is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

`N_VIsManagedMemory_Cuda`

Prototype `booleantype *N_VIsManagedMemory_Cuda(N_Vector v)`

Description This function returns a boolean flag indicating if the vector data is allocated in managed memory or not.

The NVECTOR_CUDA module defines implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. Instead, 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 [31].

The names of vector operations are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix `_Cuda` (e.g. `N_VDestroy_Cuda`). The module NVECTOR_CUDA provides the following functions:

`N_VNew_Cuda`

Single-node usage

Prototype `N_Vector N_VNew_Cuda(sunindextype length)`

Description This function creates and allocates memory for a CUDA `N_Vector`. The vector data array is allocated on both the host and device. In the *single-node* setting, the only input is the vector length. This constructor is defined in the header `nvector_cuda.h` and the library to link to is `libsundials_nveccuda`.lib.

Distributed-memory parallel usage

Prototype
```
N_Vector N_VNew_Cuda(MPI_Comm comm, sunindextype local_length,
                     sunindextype global_length)
```

Description This function creates and allocates memory for a CUDA `N_Vector`. The vector data array is allocated on both the host and device. When used in a *distributed* context with MPI, the arguments are the MPI communicator, the local vector length, and the global vector length. This constructor is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

`N_VNewManaged_Cuda`

Single-node usage

Prototype `N_Vector N_VNewManaged_Cuda(sunindextype length)`

Description This function creates and allocates memory for a CUDA `N_Vector` on a single node. The vector data array is allocated in managed memory. In the *single-node* setting, the only input is the vector length. This constructor is defined in the header `nvector_cuda.h` and the library to link to is `libsundials_nveccuda`.lib.

Distributed-memory parallel usage

Prototype
```
N_Vector N_VNewManaged_Cuda(MPI_Comm comm, sunindextype local_length,
                            sunindextype global_length)
```

Description This function creates and allocates memory for a CUDA `N_Vector` on a single node. The vector data array is allocated in managed memory. When used in a *distributed* context with MPI, the arguments are the MPI communicator, the local vector lenght, and the global vector length. This constructor is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

`N_VNewEmpty_Cuda`

Prototype `N_Vector N_VNewEmpty_Cuda()`

Description 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_VMake_Cuda`

Single-node usage

Prototype `N_Vector N_VMake_Cuda(sunindextype length, realtype *h_vdata, realtype *d_vdata)`

Description This function creates an NVECTOR_CUDA with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself. In the *single-node* setting, the inputs are the vector length, the host data array, and the device data. This constructor is defined in the header `nvector_cuda.h` and the library to link to is `libsundials_nveccuda`.lib.

Distributed-memory parallel usage

Prototype `N_Vector N_VMake_Cuda(MPI_Comm comm, sunindextype local_length, sunindextype global_length, realtype *h_vdata, realtype *d_vdata)`

Description This function creates an NVECTOR_CUDA with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself. When used in a *distributed* context with MPI, the arguments are the MPI communicator, the local vector lenght, the global vector length, the host data array, and the device data array. This constructor is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

`N_VMakeManaged_Cuda`

Single-node usage

Prototype `N_Vector N_VMakeManaged_Cuda(sunindextype length, realtype *vdata)`

Description This function creates an NVECTOR_CUDA with a user-supplied managed memory data array. This function does not allocate memory for data itself. In the *single-node* setting, the inputs are the vector length and the managed data array. This constructor is defined in the header `nvector_cuda.h` and the library to link to is `libsundials_nveccuda`.lib.

Distributed-memory parallel usage

Prototype `N_Vector N_VMakeManaged_Cuda(MPI_Comm comm, sunindextype local_length, sunindextype global_length, realtype *vdata)`

Description This function creates an NVECTOR_CUDA with a user-supplied managed memory data array. This function does not allocate memory for data itself. When used in a *distributed* context with MPI, the arguments are the MPI communicator, the local vector lenght, the global vector length, the managed data array. This constructor is defined in the header `nvector_mpicuda.h` and the library to link to is `libsundials_nvecmpicuda`.lib.

The module NVECTOR_CUDA also provides the following user-callable routines:

`N_VSetCudaStream_Cuda`

Prototype `void N_VSetCudaStream_Cuda(N_Vector v, cudaStream_t *stream)`

Description This function sets the CUDA stream that all vector kernels will be launched on. By default an NVECTOR_CUDA uses the default CUDA stream.

Note: All vectors used in a single instance of a SUNDIALS solver must use the same CUDA *stream, and the* CUDA *stream must be set prior to solver initialization. Additionally, if manually instantiating the stream and reduce* `ThreadPartitioning` *of a* `suncudavec::Vector`*, ensure that they use the same* CUDA *stream.*

`N_VCopyToDevice_Cuda`

Prototype `realtype *N_VCopyToDevice_Cuda(N_Vector v)`

Description This function copies host vector data to the device.

`N_VCopyFromDevice_Cuda`

Prototype `realtype *N_VCopyFromDevice_Cuda(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VPrint_Cuda`

Prototype `void N_VPrint_Cuda(N_Vector v)`

Description This function prints the content of a CUDA vector to `stdout`.

`N_VPrintFile_Cuda`

Prototype `void N_VPrintFile_Cuda(N_Vector v, FILE *outfile)`

Description This function prints the content of a CUDA vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_CUDA module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_Cuda`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_Cuda` will have the default settings for the NVECTOR_CUDA module.

`N_VEnableFusedOps_Cuda`

Prototype `int N_VEnableFusedOps_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Cuda`

Prototype `int N_VEnableLinearCombination_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Cuda`

Prototype `int N_VEnableScaleAddMulti_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_Cuda`

Prototype `int N_VEnableDotProdMulti_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Cuda`

Prototype `int N_VEnableLinearSumVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Cuda`

Prototype `int N_VEnableScaleVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Cuda`

Prototype `int N_VEnableConstVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the const operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormVectorArray_Cuda`

Prototype `int N_VEnableWrmsNormVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the WRMS norm operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableWrmsNormMaskVectorArray_Cuda`

Prototype `int N_VEnableWrmsNormMaskVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the masked WRMS norm operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMultiVectorArray_Cuda`

Prototype `int N_VEnableScaleAddMultiVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector array to multiple vector arrays operation in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombinationVectorArray_Cuda`

Prototype `int N_VEnableLinearCombinationVectorArray_Cuda(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

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.

7.9 The NVECTOR_RAJA implementation

The NVECTOR_RAJA module is an experimental NVECTOR implementation using the RAJA hardware abstraction layer. 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 OpenACC. 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_;
   I global_size_;
   T* h_vec_;
   T* d_vec_;
   SUNMPI_Comm comm_;
  ...
};
```

The class members are: vector size (length), size of the vector data memory block, the global vector size (length), pointers to vector data on the host and on the device, and the MPI communicator. 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 NVECTOR_RAJA module can be utilized for single-node parallelism or in a distributed context with MPI. The header file to include when using this module for single-node parallelism is `nvector_raja.h`. The header file to include when using this module in the distributed case is `nvector_mpiraja.h`. The installed module libraries to link to are `libsundials_nvecraja.`*`lib`* in the single-node case, or `libsundials_nvecmpicudaraja.`*`lib`* in the distributed case. Only one one

of these libraries may be linked to when creating an executable or library. SUNDIALS must be built with MPI support if the distributed library is desired.

7.9.1 NVECTOR_RAJA functions

Unlike other native SUNDIALS vector types, NVECTOR_RAJA does not provide macros to access its member variables. Instead, user should use the accessor functions:

`N_VGetLength_Raja`

Prototype `sunindextype N_VGetLength_Raja(N_Vector v)`

Description This function returns the global length of the vector.

`N_VGetLocalLength_Raja`

Prototype `sunindextype N_VGetLocalLength_Raja(N_Vector v)`

Description This function returns the local length of the vector.

Note: This function is for use in a *distributed context* and is defined in the header `nvector_mpiraja.h` and the library to link to is `libsundials_nvecmpicudaraja`.lib.

`N_VGetHostArrayPointer_Raja`

Prototype `realtype *N_VGetHostArrayPointer_Raja(N_Vector v)`

Description This function returns a pointer to the vector data on the host.

`N_VGetDeviceArrayPointer_Raja`

Prototype `realtype *N_VGetDeviceArrayPointer_Raja(N_Vector v)`

Description This function returns a pointer to the vector data on the device.

`N_VGetMPIComm_Raja`

Prototype `MPI_Comm N_VGetMPIComm_Raja(N_Vector v)`

Description This function returns the MPI communicator for the vector.

Note: This function is for use in a *distributed context* and is defined in the header `nvector_mpiraja.h` and the library to link to is `libsundials_nvecmpicudaraja`.lib.

The NVECTOR_RAJA module defines the implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4, except for `N_VDotProdMulti`, `N_VWrmsNormVectorArray`, and `N_VWrmsNormMaskVectorArray` as support for arrays of reduction vectors is not yet supported in RAJA. These function will be added to the NVECTOR_RAJA implementation in the future. Additionally the vector operations `N_VGetArrayPointer` and `N_VSetArrayPointer` are not implemented by the RAJA vector. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the 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 [31].

The names of vector operations are obtained from those in Tables 7.2, 7.3, and 7.4, by appending the suffix `_Raja` (e.g. `N_VDestroy_Raja`). The module NVECTOR_RAJA provides the following additional user-callable routines:

`N_VNew_Raja`

Single-node usage

Prototype `N_Vector N_VNew_Raja(sunindextype length)`

Description This function creates and allocates memory for a CUDA `N_Vector`. The vector data array is allocated on both the host and device. In the *single-node* setting, the only input is the vector length. This constructor is defined in the header `nvector_raja.h` and the library to link to is `libsundials_nveccudaraja`.lib.

Distributed-memory parallel usage

Prototype
```
N_Vector N_VNew_Raja(MPI_Comm comm, sunindextype local_length,
                     sunindextype global_length)
```

Description This function creates and allocates memory for a CUDA `N_Vector`. The vector data array is allocated on both the host and device. When used in a *distributed* context with MPI, the arguments are the MPI communicator, the local vector lenght, and the global vector length. This constructor is defined in the header `nvector_mpiraja.h` and the library to link to is `libsundials_nvecmpicudaraja`.lib.

`N_VNewEmpty_Raja`

Prototype `N_Vector N_VNewEmpty_Raja()`

Description 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_VMake_Raja`

Prototype `N_Vector N_VMake_Raja(N_VectorContent_Raja c)`

Description 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_VCopyToDevice_Raja`

Prototype `realtype *N_VCopyToDevice_Raja(N_Vector v)`

Description This function copies host vector data to the device.

`N_VCopyFromDevice_Raja`

Prototype `realtype *N_VCopyFromDevice_Raja(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VPrint_Raja`

Prototype `void N_VPrint_Raja(N_Vector v)`

Description This function prints the content of a RAJA vector to `stdout`.

`N_VPrintFile_Raja`

Prototype `void N_VPrintFile_Raja(N_Vector v, FILE *outfile)`

Description This function prints the content of a RAJA vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_RAJA module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_Raja`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_Raja` will have the default settings for the NVECTOR_RAJA module.

`N_VEnableFusedOps_Raja`

Prototype `int N_VEnableFusedOps_Raja(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the RAJA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Raja`

Prototype `int N_VEnableLinearCombination_Raja(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the RAJA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_Raja`

Prototype `int N_VEnableScaleAddMulti_Raja(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the RAJA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_Raja`

Prototype `int N_VEnableLinearSumVectorArray_Raja(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear sum operation for vector arrays in the RAJA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleVectorArray_Raja`

Prototype `int N_VEnableScaleVectorArray_Raja(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale operation for vector arrays in the RAJA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableConstVectorArray_Raja`

Prototype `int N_VEnableConstVectorArray_Raja(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the const operation for vector arrays in the RAJA vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableScaleAddMultiVectorArray_Raja

Prototype `int N_VEnableScaleAddMultiVectorArray_Raja(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale and add a vector array to multiple vector arrays operation in the RAJA vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableLinearCombinationVectorArray_Raja

Prototype
```
int N_VEnableLinearCombinationVectorArray_Raja(N_Vector v,
                                               booleantype tf)
```

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation for vector arrays in the RAJA vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

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.

7.10 The NVECTOR_OPENMPDEV implementation

In situations where a user has access to a device such as a GPU for offloading computation, SUNDIALS provides an NVECTOR implementation using OpenMP device offloading, called NVECTOR_OPENMPDEV.

The NVECTOR_OPENMPDEV implementation defines the *content* field of the N_Vector to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array on the host, a pointer to the beginning of a contiguous data array on the device, and a boolean flag own_data which specifies the ownership of host and device data arrays.

```
struct _N_VectorContent_OpenMPDEV {
  sunindextype length;
  booleantype own_data;
  realtype *host_data;
  realtype *dev_data;
};
```

The header file to include when using this module is nvector_openmpdev.h. The installed module library to link to is libsundials_nvecopenmpdev.*lib* where *.lib* is typically .so for shared libraries and .a for static libraries.

7.10.1 NVECTOR_OPENMPDEV accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMPDEV vector.

- NV_CONTENT_OMPDEV

  This routine gives access to the contents of the NVECTOR_OPENMPDEV vector N_Vector.

  The assignment v_cont = NV_CONTENT_OMPDEV(v) sets v_cont to be a pointer to the NVECTOR_OPENMPDEV N_Vector content structure.

  Implementation:

  ```
  #define NV_CONTENT_OMPDEV(v) ( (N_VectorContent_OpenMPDEV)(v->content) )
  ```

- NV_OWN_DATA_OMPDEV, NV_DATA_HOST_OMPDEV, NV_DATA_DEV_OMPDEV, NV_LENGTH_OMPDEV

  These macros give individual access to the parts of the content of an NVECTOR_OPENMPDEV N_Vector.

  The assignment v_data = NV_DATA_HOST_OMPDEV(v) sets v_data to be a pointer to the first component of the data on the host for the N_Vector v. The assignment NV_DATA_HOST_OMPDEV(v) = v_data sets the host component array of v to be v_data by storing the pointer v_data.

  The assignment v_dev_data = NV_DATA_DEV_OMPDEV(v) sets v_dev_data to be a pointer to the first component of the data on the device for the N_Vector v. The assignment NV_DATA_DEV_OMPDEV(v) = v_dev_data sets the device component array of v to be v_dev_data by storing the pointer v_dev_data.

  The assignment v_len = NV_LENGTH_OMPDEV(v) sets v_len to be the length of v. On the other hand, the call NV_LENGTH_OMPDEV(v) = len_v sets the length of v to be len_v.

  Implementation:

  ```
  #define NV_OWN_DATA_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->own_data )

  #define NV_DATA_HOST_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->host_data )

  #define NV_DATA_DEV_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->dev_data )

  #define NV_LENGTH_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->length )
  ```

7.10.2 NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 7.2, 7.3, and 7.4, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. It also provides methods for copying from the host to the device and vice versa.

The names of vector operations are obtained from those in Tables 7.2, 7.3, and 7.4 by appending the suffix _OpenMPDEV (e.g. N_VDestroy_OpenMPDEV). The module NVECTOR_OPENMPDEV provides the following additional user-callable routines:

N_VNew_OpenMPDEV

Prototype `N_Vector N_VNew_OpenMPDEV(sunindextype vec_length)`

Description This function creates and allocates memory for an NVECTOR_OPENMPDEV N_Vector.

N_VNewEmpty_OpenMPDEV

Prototype `N_Vector N_VNewEmpty_OpenMPDEV(sunindextype vec_length)`

Description This function creates a new NVECTOR_OPENMPDEV N_Vector with an empty (NULL) host and device data arrays.

`N_VMake_OpenMPDEV`

Prototype `N_Vector N_VMake_OpenMPDEV(sunindextype vec_length, realtype *h_vdata, realtype *d_vdata)`

Description This function creates an NVECTOR_OPENMPDEV vector with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself.

`N_VCloneVectorArray_OpenMPDEV`

Prototype `N_Vector *N_VCloneVectorArray_OpenMPDEV(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` NVECTOR_OPENMPDEV vectors.

`N_VCloneVectorArrayEmpty_OpenMPDEV`

Prototype `N_Vector *N_VCloneVectorArrayEmpty_OpenMPDEV(int count, N_Vector w)`

Description This function creates (by cloning) an array of `count` NVECTOR_OPENMPDEV vectors, each with an empty (`NULL`) data array.

`N_VDestroyVectorArray_OpenMPDEV`

Prototype `void N_VDestroyVectorArray_OpenMPDEV(N_Vector *vs, int count)`

Description This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_OpenMPDEV` or with `N_VCloneVectorArrayEmpty_OpenMPDEV`.

`N_VGetLength_OpenMPDEV`

Prototype `sunindextype N_VGetLength_OpenMPDEV(N_Vector v)`

Description This function returns the number of vector elements.

`N_VGetHostArrayPointer_OpenMPDEV`

Prototype `realtype *N_VGetHostArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the host data array.

`N_VGetDeviceArrayPointer_OpenMPDEV`

Prototype `realtype *N_VGetDeviceArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the device data array.

`N_VPrint_OpenMPDEV`

Prototype `void N_VPrint_OpenMPDEV(N_Vector v)`

Description This function prints the content of an NVECTOR_OPENMPDEV vector to `stdout`.

`N_VPrintFile_OpenMPDEV`

Prototype `void N_VPrintFile_OpenMPDEV(N_Vector v, FILE *outfile)`

Description This function prints the content of an NVECTOR_OPENMPDEV vector to `outfile`.

`N_VCopyToDevice_OpenMPDEV`

Prototype `void N_VCopyToDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's host data array to the device data array.

`N_VCopyFromDevice_OpenMPDEV`

Prototype `void N_VCopyFromDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's device data array to the host data array.

By default all fused and vector array operations are disabled in the NVECTOR_OPENMPDEV module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_OpenMPDEV`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with `N_VNew_OpenMPDEV` will have the default settings for the NVECTOR_OPENMPDEV module.

`N_VEnableFusedOps_OpenMPDEV`

Prototype `int N_VEnableFusedOps_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) all fused and vector array operations in the NVECTOR_OPENMPDEV vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_OpenMPDEV`

Prototype `int N_VEnableLinearCombination_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination fused operation in the NVECTOR_OPENMPDEV vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableScaleAddMulti_OpenMPDEV`

Prototype `int N_VEnableScaleAddMulti_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the scale and add a vector to multiple vectors fused operation in the NVECTOR_OPENMPDEV vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableDotProdMulti_OpenMPDEV`

Prototype `int N_VEnableDotProdMulti_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the multiple dot products fused operation in the NVECTOR_OPENMPDEV vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearSumVectorArray_OpenMPDEV`

Prototype `int N_VEnableLinearSumVectorArray_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear sum operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableScaleVectorArray_OpenMPDEV

Prototype `int N_VEnableScaleVectorArray_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableConstVectorArray_OpenMPDEV

Prototype `int N_VEnableConstVectorArray_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the const operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableWrmsNormVectorArray_OpenMPDEV

Prototype `int N_VEnableWrmsNormVectorArray_OpenMPDEV(N_Vector v, booleantype tf)`

Description This function enables (SUNTRUE) or disables (SUNFALSE) the WRMS norm operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableWrmsNormMaskVectorArray_OpenMPDEV

Prototype
```
int N_VEnableWrmsNormMaskVectorArray_OpenMPDEV(N_Vector v,
                                               booleantype tf)
```

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableScaleAddMultiVectorArray_OpenMPDEV

Prototype
```
int N_VEnableScaleAddMultiVectorArray_OpenMPDEV(N_Vector v,
                                                booleantype tf)
```

Description This function enables (SUNTRUE) or disables (SUNFALSE) the scale and add a vector array to multiple vector arrays operation in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableLinearCombinationVectorArray_OpenMPDEV

Prototype
```
int N_VEnableLinearCombinationVectorArray_OpenMPDEV(N_Vector v,
                                                    booleantype tf)
```

Description This function enables (SUNTRUE) or disables (SUNFALSE) the linear combination operation for vector arrays in the NVECTOR_OPENMPDEV vector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

Notes

- When looping over the components of an `N_Vector v`, it is most efficient to first obtain the component array via `h_data = NV_DATA_HOST_OMPDEV(v)` for the host array or `d_data = NV_DATA_DEV_OMPDEV(v)` for the device array and then access `h_data[i]` or `d_data[i]` within the loop.
- When accessing individual components of an `N_Vector v` on the host remember to first copy the array back from the device with `N_VCopyFromDevice_OpenMPDEV(v)` to ensure the array is up to date.

- `N_VNewEmpty_OpenMPDEV`, `N_VMake_OpenMPDEV`, and `N_VCloneVectorArrayEmpty_OpenMPDEV` set the field `own_data` = `SUNFALSE`. `N_VDestroy_OpenMPDEV` and `N_VDestroyVectorArray_OpenMPDEV` will not attempt to free the pointer *data* for any `N_Vector` with `own_data` set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_OPENMPDEV 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.

7.11 NVECTOR Examples

There are `NVector` examples that may be installed for the implementations provided with SUNDIALS. 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 the max norm.
- `Test_N_VWrmsNorm`: Create vector of known values, find and validate the weighted root mean square.
- `Test_N_VWrmsNormMask`: Create vector of known values, find and validate the weighted root mean square using all elements except one.
- `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.
- `Test_N_VLinearCombination` Case 1a: Test x = a x
- `Test_N_VLinearCombination` Case 1b: Test z = a x
- `Test_N_VLinearCombination` Case 2a: Test x = a x + b y
- `Test_N_VLinearCombination` Case 2b: Test z = a x + b y

- `Test_N_VLinearCombination` Case 3a: Test x = x + a y + b z
- `Test_N_VLinearCombination` Case 3b: Test x = a x + b y + c z
- `Test_N_VLinearCombination` Case 3c: Test w = a x + b y + c z
- `Test_N_VScaleAddMulti` Case 1a: y = a x + y
- `Test_N_VScaleAddMulti` Case 1b: z = a x + y
- `Test_N_VScaleAddMulti` Case 2a: Y[i] = c[i] x + Y[i], i = 1,2,3
- `Test_N_VScaleAddMulti` Case 2b: Z[i] = c[i] x + Y[i], i = 1,2,3
- `Test_N_VDotProdMulti` Case 1: Calculate the dot product of two vectors
- `Test_N_VDotProdMulti` Case 2: Calculate the dot product of one vector with three other vectors in a vector array.
- `Test_N_VLinearSumVectorArray` Case 1: z = a x + b y
- `Test_N_VLinearSumVectorArray` Case 2a: Z[i] = a X[i] + b Y[i]
- `Test_N_VLinearSumVectorArray` Case 2b: X[i] = a X[i] + b Y[i]
- `Test_N_VLinearSumVectorArray` Case 2c: Y[i] = a X[i] + b Y[i]
- `Test_N_VScaleVectorArray` Case 1a: y = c y
- `Test_N_VScaleVectorArray` Case 1b: z = c y
- `Test_N_VScaleVectorArray` Case 2a: Y[i] = c[i] Y[i]
- `Test_N_VScaleVectorArray` Case 2b: Z[i] = c[i] Y[i]
- `Test_N_VScaleVectorArray` Case 1a: z = c
- `Test_N_VScaleVectorArray` Case 1b: Z[i] = c
- `Test_N_VWrmsNormVectorArray` Case 1a: Create a vector of know values, find and validate the weighted root mean square norm.
- `Test_N_VWrmsNormVectorArray` Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each.
- `Test_N_VWrmsNormMaskVectorArray` Case 1a: Create a vector of know values, find and validate the weighted root mean square norm using all elements except one.
- `Test_N_VWrmsNormMaskVectorArray` Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each using all elements except one.
- `Test_N_VScaleAddMultiVectorArray` Case 1a: y = a x + y
- `Test_N_VScaleAddMultiVectorArray` Case 1b: z = a x + y
- `Test_N_VScaleAddMultiVectorArray` Case 2a: Y[j][0] = a[j] X[0] + Y[j][0]
- `Test_N_VScaleAddMultiVectorArray` Case 2b: Z[j][0] = a[j] X[0] + Y[j][0]
- `Test_N_VScaleAddMultiVectorArray` Case 3a: Y[0][i] = a[0] X[i] + Y[0][i]
- `Test_N_VScaleAddMultiVectorArray` Case 3b: Z[0][i] = a[0] X[i] + Y[0][i]

- `Test_N_VScaleAddMultiVectorArray` Case 4a: Y[j][i] = a[j] X[i] + Y[j][i]
- `Test_N_VScaleAddMultiVectorArray` Case 4b: Z[j][i] = a[j] X[i] + Y[j][i]
- `Test_N_VLinearCombinationVectorArray` Case 1a: x = a x
- `Test_N_VLinearCombinationVectorArray` Case 1b: z = a x
- `Test_N_VLinearCombinationVectorArray` Case 2a: x = a x + b y
- `Test_N_VLinearCombinationVectorArray` Case 2b: z = a x + b y
- `Test_N_VLinearCombinationVectorArray` Case 3a: x = a x + b y + c z
- `Test_N_VLinearCombinationVectorArray` Case 3b: w = a x + b y + c z
- `Test_N_VLinearCombinationVectorArray` Case 4a: X[0][i] = c[0] X[0][i]
- `Test_N_VLinearCombinationVectorArray` Case 4b: Z[i] = c[0] X[0][i]
- `Test_N_VLinearCombinationVectorArray` Case 5a: X[0][i] = c[0] X[0][i] + c[1] X[1][i]
- `Test_N_VLinearCombinationVectorArray` Case 5b: Z[i] = c[0] X[0][i] + c[1] X[1][i]
- `Test_N_VLinearCombinationVectorArray` Case 6a: X[0][i] = X[0][i] + c[1] X[1][i] + c[2] X[2][i]
- `Test_N_VLinearCombinationVectorArray` Case 6b: X[0][i] = c[0] X[0][i] + c[1] X[1][i] + c[2] X[2][i]
- `Test_N_VLinearCombinationVectorArray` Case 6c: Z[i] = c[0] X[0][i] + c[1] X[1][i] + c[2] X[2][i]

Table 7.5: List of vector functions usage by IDAS code modules

	IDAS	IDALS	IDABBDPRE	IDAA
N_VGetVectorID				
N_VClone	✓	✓	✓	✓
N_VCloneEmpty		1		
N_VDestroy	✓	✓	✓	✓
N_VCloneVectorArray	✓			✓
N_VDestroyVectorArray	✓			✓
N_VSpace	✓	2		
N_VGetArrayPointer		1	✓	
N_VSetArrayPointer		1		
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	✓			
N_VLinearCombination	✓			
N_VScaleAddMulti	✓			
N_VDotProdMulti		3		
N_VLinearSumVectorArray	✓			
N_VScaleVectorArray	✓			
N_VConstVectorArray	✓			
N_VWrmsNormVectorArray	✓			
N_VWrmsNormMaskVectorArray	✓			
N_VScaleAddMultiVectorArray	✓			
N_VLinearCombinationVectorArray	✓			

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 × N matrix	0
SUNMATRIX_BAND	Band M × M matrix	1
SUNMATRIX_SPARSE	Sparse (CSR or CSC) M × 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 SUNMatrix functions used by IDAS

In Table 8.4, 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. The main IDAS integrator does not call any SUNMATRIX functions directly, so the table columns are specific to the IDALS interface and the IDABBDPRE preconditioner module. We further note that the IDALS interface only utilizes these routines when supplied with a *matrix-based* linear solver, i.e., the SUNMATRIX object passed to `IDASetLinearSolver` was not `NULL`.

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

	IDALS	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.

8.2 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 include when using this module is `sunmatrix/sunmatrix_dense.h`. The SUNMATRIX_DENSE module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixdense` module library.

8.2.1 SUNMatrix_Dense accessor macros

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] )
```

8.2.2 SUNMatrix_Dense functions

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). All the standard matrix operations listed in 8.2 with the suffix _Dense appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Dense).

The module SUNMATRIX_DENSE provides the following additional user-callable routines:

SUNDenseMatrix

Prototype `SUNMatrix SUNDenseMatrix(sunindextype M, sunindextype N)`

Description 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.

F2003 Name This function is callable as FSUNDenseMatrix when using the Fortran 2003 interface module.

SUNDenseMatrix_Print

Prototype `void SUNDenseMatrix_Print(SUNMatrix A, FILE* outfile)`

Description 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.

SUNDenseMatrix_Rows

Prototype `sunindextype SUNDenseMatrix_Rows(SUNMatrix A)`

Description This function returns the number of rows in the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix_Rows when using the Fortran 2003 interface module.

SUNDenseMatrix_Columns

Prototype `sunindextype SUNDenseMatrix_Columns(SUNMatrix A)`

Description This function returns the number of columns in the dense SUNMatrix.

F2003 Name This function is callable as FSUNDenseMatrix_Columns when using the Fortran 2003 interface module.

`SUNDenseMatrix_LData`

Prototype `sunindextype SUNDenseMatrix_LData(SUNMatrix A)`

Description This function returns the length of the data array for the dense `SUNMatrix`.

F2003 Name This function is callable as `FSUNDenseMatrix_LData` when using the Fortran 2003 interface module.

`SUNDenseMatrix_Data`

Prototype `realtype* SUNDenseMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the dense `SUNMatrix`.

F2003 Name This function is callable as `FSUNDenseMatrix_Data` when using the Fortran 2003 interface module.

`SUNDenseMatrix_Cols`

Prototype `realtype** SUNDenseMatrix_Cols(SUNMatrix A)`

Description This function returns a pointer to the cols array for the dense `SUNMatrix`.

`SUNDenseMatrix_Column`

Prototype `realtype* SUNDenseMatrix_Column(SUNMatrix A, sunindextype j)`

Description 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 $\texttt{M} - 1$.

F2003 Name This function is callable as `FSUNDenseMatrix_Column` when using the Fortran 2003 interface module.

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.

8.2.3 SUNMatrix_Dense Fortran interfaces

The SUNMATRIX_DENSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunmatrix_dense_mod` FORTRAN module defines interfaces to most SUNMATRIX_DENSE C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNDenseMatrix` is interfaced as `FSUNDenseMatrix`.

The FORTRAN 2003 SUNMATRIX_DENSE interface module can be accessed with the `use` statement, i.e. `use fsunmatrix_dense_mod`, and linking to the library `libsundials_fsunmatrixdense_mod.lib` in addition to the C library. For details on where the library and module file `fsunmatrix_dense_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunmatrixdense_mod` library.

FORTRAN 77 interface functions

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.

8.3 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`+`ml`+1)

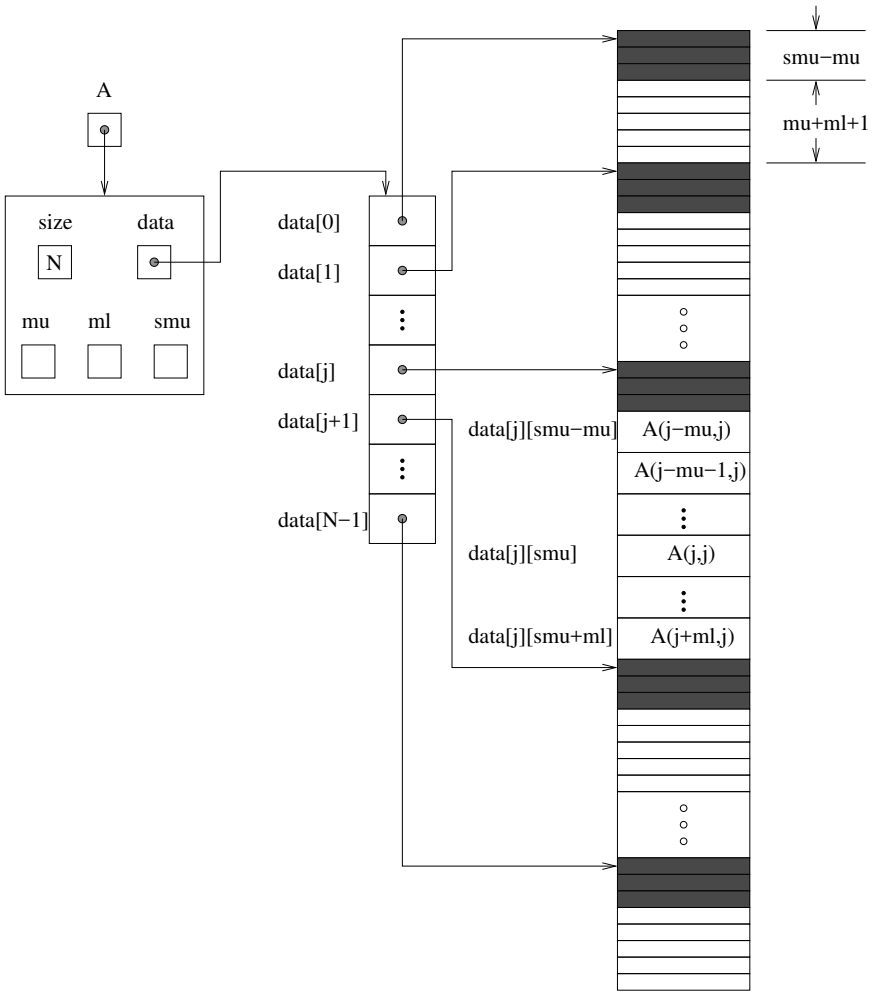

Figure 8.1: Diagram of the storage for the SUNMATRIX_BAND module. Here `A` is an `N` × `N` band matrix with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to `N` − 1 and the (i, j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the associated SUNLINSOL_BAND linear solver.

`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`·N)

`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` $\le i \le j$+`ml`.

The header file to include when using this module is `sunmatrix/sunmatrix_band.h`. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixband` module library.

8.3.1 SUNMatrix_Band accessor macros

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.

  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 ≤ i ≤ 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)] )
```

8.3.2 SUNMatrix_Band functions

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). All the standard matrix operations listed in 8.2 with the suffix _Band appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Band).

The module SUNMATRIX_BAND provides the following additional user-callable routines:

SUNBandMatrix

Prototype `SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu, sunindextype ml)`

Description This constructor function creates and allocates memory for a banded SUNMatrix. Its arguments are the matrix size, N, and the upper and lower half-bandwidths of the matrix, mu and ml. The stored upper bandwidth is set to mu+ml to accommodate subsequent factorization in the SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules.

F2003 Name This function is callable as FSUNBandMatrix when using the Fortran 2003 interface module.

SUNBandMatrixStorage

Prototype `SUNMatrix SUNBandMatrixStorage(sunindextype N, sunindextype mu,`
`sunindextype ml, sunindextype smu)`

Description 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, this value should be

- at least min(N-1,mu+ml) if the matrix will be used by the SUNLINSOL_BAND module;
- exactly equal to mu+ml if the matrix will be used by the SUNLINSOL_LAPACKBAND module;
- at least mu if used in some other manner.

Note: it is strongly recommended that users call the default constructor, SUNBandMatrix*, in all standard use cases. This advanced constructor is used internally within* SUNDIALS *solvers, and is provided to users who require banded matrices for non-default purposes.*

`SUNBandMatrix_Print`

Prototype `void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile)`

Description 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.

`SUNBandMatrix_Rows`

Prototype `sunindextype SUNBandMatrix_Rows(SUNMatrix A)`

Description This function returns the number of rows in the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_Rows` when using the Fortran 2003 interface module.

`SUNBandMatrix_Columns`

Prototype `sunindextype SUNBandMatrix_Columns(SUNMatrix A)`

Description This function returns the number of columns in the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_Columns` when using the Fortran 2003 interface module.

`SUNBandMatrix_LowerBandwidth`

Prototype `sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A)`

Description This function returns the lower half-bandwidth of the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_LowerBandwidth` when using the Fortran 2003 interface module.

`SUNBandMatrix_UpperBandwidth`

Prototype `sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A)`

Description This function returns the upper half-bandwidth of the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_UpperBandwidth` when using the Fortran 2003 interface module.

`SUNBandMatrix_StoredUpperBandwidth`

Prototype `sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A)`

Description This function returns the stored upper half-bandwidth of the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_StoredUpperBandwidth` when using the Fortran 2003 interface module.

`SUNBandMatrix_LDim`

Prototype `sunindextype SUNBandMatrix_LDim(SUNMatrix A)`

Description This function returns the length of the leading dimension of the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_LDim` when using the Fortran 2003 interface module.

`SUNBandMatrix_Data`

Prototype `realtype* SUNBandMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the banded `SUNMatrix`.

F2003 Name This function is callable as `FSUNBandMatrix_Data` when using the Fortran 2003 interface module.

`SUNBandMatrix_Cols`

Prototype `realtype** SUNBandMatrix_Cols(SUNMatrix A)`

Description This function returns a pointer to the cols array for the banded `SUNMatrix`.

`SUNBandMatrix_Column`

Prototype `realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j)`

Description 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`.

F2003 Name This function is callable as `FSUNBandMatrix_Column` when using the Fortran 2003 interface module.

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.

8.3.3 SUNMatrix_Band Fortran interfaces

The SUNMATRIX_BAND module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunmatrix_band_mod` FORTRAN module defines interfaces to most SUNMATRIX_BAND C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNBandMatrix` is interfaced as `FSUNBandMatrix`.

The FORTRAN 2003 SUNMATRIX_BAND interface module can be accessed with the `use` statement, i.e. `use fsunmatrix_band_mod`, and linking to the library `libsundials_fsunmatrixband_mod.`*lib* in

addition to the C library. For details on where the library and module file `fsunmatrix_band_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunmatrixband_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the SUNMATRIX_BAND module also includes the FORTRAN-callable function `FSUNBandMatInit(code, N, mu, ml, 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`, and `ml` 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, ier)` initializes this SUNMATRIX_BAND module for storing the mass matrix.

8.4 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};
```

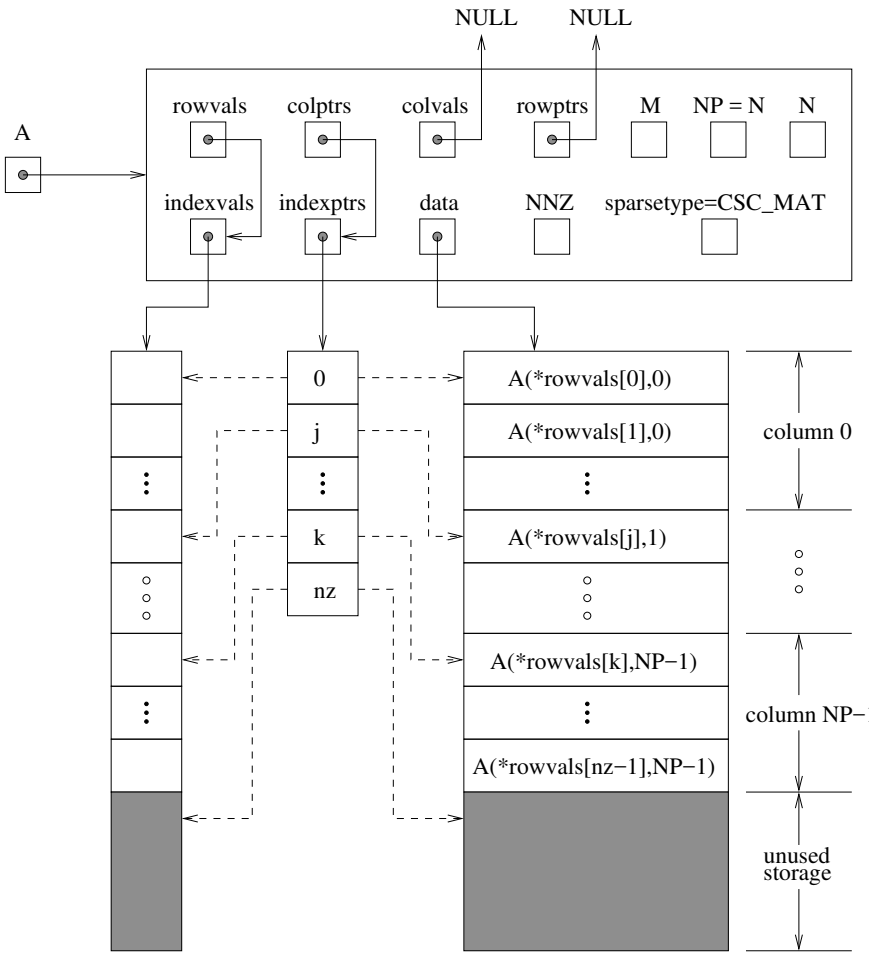

Figure 8.2: Diagram of the storage for a compressed-sparse-column matrix. Here `A` is an $\texttt{M} \times \texttt{N}$ sparse matrix with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to $\texttt{M} - 1$, 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.

The header file to include when using this module is `sunmatrix/sunmatrix_sparse.h`. The SUNMATRIX_SPARSE module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixsparse` module library.

8.4.1 SUNMatrix_Sparse accessor macros

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`.

  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 )
  ```

8.4.2 SUNMatrix_Sparse functions

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`). All the standard matrix operations listed in 8.2 with the suffix `_Sparse` appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. `FSUNMatCopy_Sparse`).

The module SUNMATRIX_SPARSE provides the following additional user-callable routines:

`SUNSparseMatrix`

Prototype
```
SUNMatrix SUNSparseMatrix(sunindextype M, sunindextype N,
                          sunindextype NNZ, int sparsetype)
```

Description 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`).

F2003 Name This function is callable as `FSUNSparseMatrix` when using the Fortran 2003 interface module.

`SUNSparseFromDenseMatrix`

Prototype
```
SUNMatrix SUNSparseFromDenseMatrix(SUNMatrix A, realtype droptol,
                                   int sparsetype);
```

Description 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.

F2003 Name This function is callable as `FSUNSparseFromDenseMatrix` when using the Fortran 2003 interface module.

`SUNSparseFromBandMatrix`

Prototype
```
SUNMatrix SUNSparseFromBandMatrix(SUNMatrix A, realtype droptol,
                                  int sparsetype);
```

Description 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.

F2003 Name This function is callable as `FSUNSparseFromBandMatrix` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Realloc`

Prototype `int SUNSparseMatrix_Realloc(SUNMatrix A)`

Description 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).

F2003 Name This function is callable as `FSUNSparseMatrix_Realloc` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Reallocate`

Prototype `int SUNSparseMatrix_Reallocate(SUNMatrix A, sunindextype NNZ)`

Description This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has storage for a specified number of nonzeros. Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse or if NNZ is negative).

F2003 Name This function is callable as `FSUNSparseMatrix_Reallocate` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Print`

Prototype `void SUNSparseMatrix_Print(SUNMatrix A, FILE* outfile)`

Description 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.

`SUNSparseMatrix_Rows`

Prototype `sunindextype SUNSparseMatrix_Rows(SUNMatrix A)`

Description This function returns the number of rows in the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_Rows` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Columns`

Prototype `sunindextype SUNSparseMatrix_Columns(SUNMatrix A)`

Description This function returns the number of columns in the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_Columns` when using the Fortran 2003 interface module.

`SUNSparseMatrix_NNZ`

Prototype `sunindextype SUNSparseMatrix_NNZ(SUNMatrix A)`

Description This function returns the number of entries allocated for nonzero storage for the sparse matrix `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_NNZ` when using the Fortran 2003 interface module.

`SUNSparseMatrix_NP`

Prototype `sunindextype SUNSparseMatrix_NP(SUNMatrix A)`

Description 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.

F2003 Name This function is callable as `FSUNSparseMatrix_NP` when using the Fortran 2003 interface module.

`SUNSparseMatrix_SparseType`

Prototype `int SUNSparseMatrix_SparseType(SUNMatrix A)`

Description This function returns the storage type (`CSR_MAT` or `CSC_MAT`) for the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_SparseType` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Data`

Prototype `realtype* SUNSparseMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_Data` when using the Fortran 2003 interface module.

`SUNSparseMatrix_IndexValues`

Prototype `sunindextype* SUNSparseMatrix_IndexValues(SUNMatrix A)`

Description 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.

F2003 Name This function is callable as `FSUNSparseMatrix_IndexValues` when using the Fortran 2003 interface module.

`SUNSparseMatrix_IndexPointers`

Prototype `sunindextype* SUNSparseMatrix_IndexPointers(SUNMatrix A)`

Description 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.

F2003 Name This function is callable as `FSUNSparseMatrix_IndexPointers` when using the Fortran 2003 interface module.

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.

8.4.3 SUNMatrix_Sparse Fortran interfaces

The SUNMATRIX_SPARSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunmatrix_sparse_mod` FORTRAN module defines interfaces to most SUNMATRIX_SPARSE C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNSparseMatrix` is interfaced as `FSUNSparseMatrix`.

The FORTRAN 2003 SUNMATRIX_SPARSE interface module can be accessed with the `use` statement, i.e. `use fsunmatrix_sparse_mod`, and linking to the library `libsundials_fsunmatrixsparse_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunmatrix_sparse_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunmatrixsparse_mod` library.

FORTRAN 77 interface functions

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.

Chapter 9

Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS packages operate using generic linear solver modules defined through the SUNLINSOL API. This allows SUNDIALS packages to utilize any valid SUNLINSOL implementation that provides a set of required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group consists of "set" routines to supply the linear solver object with functions provided by the SUNDIALS package, or for modification of solver parameters. The last group consists of "get" routines for retrieving artifacts (statistics, residual vectors, etc.) from the linear solver. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

The implementations provided with SUNDIALS 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 (matrix-based or matrix-free) methods. Moreover, advanced users can provide a customized `SUNLinearSolver` implementation to any SUNDIALS package, particularly in cases where they provide their own NVECTOR and/or SUNMATRIX modules.

Historically, the SUNDIALS packages have been designed to specifically leverage the use of either *direct linear solvers* or matrix-free, *scaled, preconditioned, iterative linear solvers*. However, matrix-based iterative linear solvers are also supported.

The iterative linear solvers packaged with SUNDIALS 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, these 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 $P_2 x$.

SUNDIALS packages request that iterative linear solvers stop based on the 2-norm of the scaled preconditioned residual meeting a prescribed tolerance

$$\left\|\tilde{b} - \tilde{A}\tilde{x}\right\|_2 < \text{tol}.$$

When provided an iterative SUNLINSOL implementation that does not support the scaling matrices S_1 and S_2, SUNDIALS' packages will adjust the value of tol accordingly (see §9.4.2 for more details). In this case, they instead request that iterative linear solvers stop based on the criteria

$$\left\|P_1^{-1}b - P_1^{-1}Ax\right\|_2 < \text{tol}.$$

We note that the corresponding adjustments to tol in this case are non-optimal, in that they cannot balance error between specific entries of the solution x, only the aggregate error in the overall solution vector.

We further note that not all of the SUNDIALS-provided iterative linear solvers support the full range of the above options (e.g., separate left/right preconditioning), and that some of the SUNDIALS packages only utilize a subset of these options. Further details on these exceptions are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS package.

For users interested in providing their own SUNLINSOL module, the following section presents the SUNLINSOL API and its implementation beginning with the definition of SUNLINSOL functions in sections 9.1.1 – 9.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 9.1.4. A table of linear solver return codes is given in section 9.1.5. The `SUNLinearSolver` type and the generic SUNLINSOL module are defined in section 9.1.6. The section 9.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 9.3 lists the requirements for supplying a custom SUNLINSOL module and discusses some intended use cases. Users wishing to supply their own SUNLINSOL module are encouraged to use the SUNLINSOL implementations provided with SUNDIALS as a template for supplying custom linear solver modules. The SUNLINSOL functions required by this SUNDIALS package as well as other package specific details are given in section 9.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

9.1 The SUNLinearSolver API

The SUNLINSOL API defines several linear solver operations that enable SUNDIALS packages to utilize any SUNLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group of functions consists of set routines to supply the linear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving linear solver statistics. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

9.1.1 SUNLinearSolver core functions

The core linear solver functions consist of four required routines to get the linear solver type (`SUNLinSolGetType`), initialize the linear solver object once all solver-specific options have been set (`SUNLinSolInitialize`), set up the linear solver object to utilize an updated matrix A (`SUNLinSolSetup`), and solve the linear system $Ax = b$ (`SUNLinSolSolve`). The remaining routine for destruction of the linear solver object (`SUNLinSolFree`) is optional.

`SUNLinSolGetType`

Call `type = SUNLinSolGetType(LS);`

Description The *required* function `SUNLinSolGetType` returns the type identifier for the linear solver `LS`. It is used to determine the solver type (direct, iterative, or matrix-iterative) from the abstract `SUNLinearSolver` interface.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

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

- `SUNLINEARSOLVER_DIRECT` – `0`, the SUNLINSOL module requires a matrix, and computes an 'exact' solution to the linear system defined by that matrix.
- `SUNLINEARSOLVER_ITERATIVE` – `1`, the SUNLINSOL module does not require a matrix (though one may be provided), and computes an inexact solution to the linear system using a matrix-free iterative algorithm. That is it solves the linear system defined by the package-supplied `ATimes` routine (see `SUNLinSolSetATimes` below), even if that linear system differs from the one encoded in the matrix object (if one is provided). As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.
- `SUNLINEARSOLVER_MATRIX_ITERATIVE` – `2`, the SUNLINSOL module requires a matrix, and computes an inexact solution to the linear system defined by that matrix using an iterative algorithm. That is it solves the linear system defined by the matrix object even if that linear system differs from that encoded by the package-supplied `ATimes` routine. As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.

Notes See section 9.3.1 for more information on intended use cases corresponding to the linear solver type.

`SUNLinSolInitialize`

Call `retval = SUNLinSolInitialize(LS);`

Description The *required* function `SUNLinSolInitialize` performs linear solver initialization (assuming that all solver-specific options have been set).

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value 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 9.1.

`SUNLinSolSetup`

Call `retval = SUNLinSolSetup(LS, A);`

Description The *required* function `SUNLinSolSetup` 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.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`A` (`SUNMatrix`) a SUNMATRIX object.

Return value 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 9.1.

`SUNLinSolSolve`

Call `retval = SUNLinSolSolve(LS, A, x, b, tol);`

Description The *required* function `SUNLinSolSolve` solves a linear system $Ax = b$.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`A` (`SUNMatrix`) a SUNMATRIX object.

`x` (`N_Vector`) a NVECTOR object containing the initial guess for the solution of the linear system, and the solution to the linear system upon return.

`b` (`N_Vector`) a NVECTOR object containing the linear system right-hand side.

`tol` (`realtype`) the desired linear solver tolerance.

Return value 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 9.1.

Notes **Direct solvers:** can ignore the `tol` argument.

Matrix-free solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE`) can ignore the SUNMATRIX input `A`, and should instead rely on the matrix-vector product function supplied through the routine `SUNLinSolSetATimes`.

Iterative solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`) should attempt to solve to the specified tolerance `tol` in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.

`SUNLinSolFree`

Call `retval = SUNLinSolFree(LS);`

Description The *optional* function `SUNLinSolFree` frees memory allocated by the linear solver.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value This should return zero for a successful call and a negative value for a failure.

9.1.2 SUNLinearSolver set functions

The following set functions are used to supply linear solver modules with functions defined by the SUNDIALS packages and to modify solver parameters. Only the routine for setting the matrix-vector product routine is required, and that is only for matrix-free linear solver modules. Otherwise, all other set functions are optional. SUNLINSOL implementations that do not provide the functionality for any optional routine should leave the corresponding function pointer `NULL` instead of supplying a dummy routine.

`SUNLinSolSetATimes`

Call `retval = SUNLinSolSetATimes(LS, A_data, ATimes);`

Description The function `SUNLinSolSetATimes` is *required for matrix-free linear solvers*; otherwise it is optional.

This routine provides an `ATimesFn` function pointer, as well as a `void*` pointer to a data structure used by this routine, to a linear solver object. SUNDIALS packages 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.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`A_data` (`void*`) data structure passed to `ATimes`.

`ATimes` (`ATimesFn`) function pointer implementing the matrix-vector product routine.

Return value 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 9.1.

`SUNLinSolSetPreconditioner`

Call `retval = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);`

Description The *optional* function `SUNLinSolSetPreconditioner` 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 package, which will provide translation between the generic `Pset` and `Psol` calls and the package- or user-supplied routines.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`Pdata` (`void*`) data structure passed to both `Pset` and `Psol`.
`Pset` (`PSetupFn`) function pointer implementing the preconditioner setup.
`Psol` (`PSolveFn`) function pointer implementing the preconditioner solve.

Return value 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 9.1.

`SUNLinSolSetScalingVectors`

Call `retval = SUNLinSolSetScalingVectors(LS, s1, s2);`

Description The *optional* function `SUNLinSolSetScalingVectors` provides left/right scaling vectors for the linear system solve. Here, `s1` and `s2` are NVECTOR of positive scale factors containing the diagonal of the matrices S_1 and S_2 from equations (9.1)-(9.2), respectively. Neither of these vectors need to be tested for positivity, and a `NULL` argument for either indicates that the corresponding scaling matrix is the identity.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`s1` (`N_Vector`) diagonal of the matrix S_1
`s2` (`N_Vector`) diagonal of the matrix S_2

Return value 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 9.1.

9.1.3 SUNLinearSolver get functions

The following get functions allow SUNDIALS packages to retrieve results from a linear solve. All routines are optional.

`SUNLinSolNumIters`

Call `its = SUNLinSolNumIters(LS);`

Description The *optional* function `SUNLinSolNumIters` should return the number of linear iterations performed in the last 'solve' call.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value `int` containing the number of iterations

`SUNLinSolResNorm`

Call `rnorm = SUNLinSolResNorm(LS);`

Description The *optional* function `SUNLinSolResNorm` should return the final residual norm from the last 'solve' call.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value `realtype` containing the final residual norm

`SUNLinSolResid`

Call `rvec = SUNLinSolResid(LS);`

Description 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 *optional* routine may be called by the SUNDIALS package. This routine should return the NVECTOR containing the preconditioned initial residual vector.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value `N_Vector` containing the final residual vector

Notes Since `N_Vector` is actually a pointer, and the results are not modified, this routine should *not* require additional memory allocation. If the SUNLINSOL object does not retain a vector for this purpose, then this function pointer should be set to `NULL` in the implementation.

`SUNLinSolLastFlag`

Call `lflag = SUNLinSolLastFlag(LS);`

Description The *optional* function `SUNLinSolLastFlag` should return the last error flag encountered within the linear solver. This is not called by the SUNDIALS packages directly; it allows the user to investigate linear solver issues after a failed solve.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value `long int` containing the most recent error flag

`SUNLinSolSpace`

Call `retval = SUNLinSolSpace(LS, &lrw, &liw);`

Description The *optional* function `SUNLinSolSpace` should return the storage requirements for the linear solver `LS`.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`lrw` (`long int*`) the number of realtype words stored by the linear solver.

`liw` (`long int*`) the number of integer words stored by the linear solver.

Return value 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 9.1.

Notes This function is advisory only, for use in determining a user's total space requirements.

9.1.4 Functions provided by SUNDIALS packages

To interface with the SUNLINSOL modules, the SUNDIALS packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic interfaces to the linear systems of equations that result in their solution. The types for functions provided to a SUNLINSOL module are defined in the header file `sundials/sundials_iterative.h`, and are described below.

`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.

`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.

`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.

9.1.5 `SUNLinearSolver` return codes

The functions provided to SUNLINSOL modules by each SUNDIALS package, and functions within the SUNDIALS-provided SUNLINSOL implementations utilize a common set of return codes, shown in Table 9.1. These adhere to a common pattern: 0 indicates success, a postitive value corresponds to a recoverable failure, and a negative value indicates a non-recoverable failure. Aside from this pattern, the actual values of each error code are primarily to provide additional information to the user in case of a linear solver failure.

Table 9.1: 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)
SUNLS_LUFACT_FAIL	8	a singular matrix was encountered during a LU factorization (SUNLINSOL_DENSE/SUNLINSOL_BAND)

9.1.6 The generic SUNLinearSolver module

SUNDIALS packages interact with specific SUNLINSOL implementations through the generic SUNLINSOL module on which all other SUNLINSOL iplementations are built. The SUNLinearSolver type is a pointer to a structure containing an implementation-dependent *content* field, and an *ops* field. The type SUNLinearSolver is defined as

```
typedef struct _generic_SUNLinearSolver *SUNLinearSolver;

struct _generic_SUNLinearSolver {
  void *content;
  struct _generic_SUNLinearSolver_Ops *ops;
};
```

where the _generic_SUNLinearSolver_Ops structure is a list of pointers to the various actual linear solver operations provided by a specific implementation. The _generic_SUNLinearSolver_Ops structure 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 defined in Sections 9.1.1-9.1.3. These routines are in fact only wrappers to 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));
}
```

9.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 9.2 we show the matrix-based 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 9.2: SUNDIALS matrix-based 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	✓	✓	✓	✓

9.3 Implementing a custom SUNLinearSolver module

A particular implementation of the SUNLINSOL module must:

- Specify the *content* field of the `SUNLinearSolver` object.
- Define and implement a minimal subset of the linear solver operations. See the section 9.4 to determine which SUNLINSOL operations are required for this SUNDIALS package.

  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.

We note that the function pointers for all unsupported optional routines should be set to `NULL` in the *ops* structure. This allows the SUNDIALS package that is using the SUNLINSOL object to know that the associated functionality is not supported.

Additionally, a SUNLINSOL implementation *may* do the following:

- Define and implement additional user-callable "set" routines acting on the `SUNLinearSolver`, e.g., for setting various configuration options to tune the linear solver to a particular problem.
- Provide additional user-callable "get" routines acting on the `SUNLinearSolver` object, e.g., for returning various solve statistics.

9.3.1 Intended use cases

The SUNLINSOL (and SUNMATRIX) APIs are designed to require a minimal set of routines to ease interfacing with custom or third-party linear solver libraries. External solvers provide similar routines with the necessary functionality and thus will require minimal effort to wrap within custom SUNMATRIX and SUNLINSOL implementations. Sections 8.1 and 9.4 include a list of the required set of routines that compatible SUNMATRIX and SUNLINSOL implementations must provide. As SUNDIALS packages utilize generic SUNLINSOL modules allowing for user-supplied `SUNLinearSolver` implementations, there exists a wide range of possible linear solver combinations. Some intended use cases for both the SUNDIALS-provided and user-supplied SUNLINSOL modules are discussd in the following sections.

Direct linear solvers

Direct linear solver modules require a matrix and compute an 'exact' solution to the linear system *defined by the matrix*. Multiple matrix formats and associated direct linear solvers are supplied with SUNDIALS through different SUNMATRIX and SUNLINSOL implementations. SUNDIALS packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations. As a result, each package's linear solver interface recomputes Jacobian information as infrequently as possible.

Alternative matrix storage formats and compatible linear solvers that are not currently provided by, or interfaced with, SUNDIALS can leverage this infrastructure with minimal effort. To do so, a user must implement custom SUNMATRIX and SUNLINSOL wrappers for the desired matrix format and/or linear solver following the APIs described in Chapters 8 and 9. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_DIRECT` *type.*

Matrix-free iterative linear solvers

Matrix-free iterative linear solver modules do not require a matrix and compute an inexact solution to the linear system *defined by the package-supplied* `ATimes` *routine*. SUNDIALS supplies multiple scaled, preconditioned iterative linear solver (spils) SUNLINSOL modules that support scaling to allow users to handle non-dimensionalization (as best as possible) within each SUNDIALS package and retain variables and define equations as desired in their applications. For linear solvers that do not support left/right scaling, the tolerance supplied to the linear solver is adjusted to compensate (see section 9.4.2 for

more details); however, this use case may be non-optimal and cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single problem.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, SUNDIALS a user must implement a custom SUNLINSOL wrapper for the linear solver following the API described in Chapter 9. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_ITERATIVE` *type.*

Matrix-based iterative linear solvers (reusing A)

Matrix-based iterative linear solver modules require a matrix and compute an inexact solution to the linear system *defined by the matrix*. This matrix will be updated infrequently and resued across multiple solves to amortize cost of matrix construction. As in the direct linear solver case, only wrappers for the matrix and linear solver in SUNMATRIX and SUNLINSOL implementations need to be created to utilize a new linear solver. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_MATRIX_ITERATIVE` *type.*

At present, SUNDIALS has one example problem that uses this approach for wrapping a structured-grid matrix, linear solver, and preconditioner from the *hypre* library that may be used as a template for other customized implementations (see `examples/arkode/CXX_parhyp/ark_heat2D_hypre.cpp`).

Matrix-based iterative linear solvers (current A)

For users who wish to utilize a matrix-based iterative linear solver module where the matrix is *purely for preconditioning* and the linear system is *defined by the package-supplied* `ATimes` *routine*, we envision two current possibilities.

The preferred approach is for users to employ one of the SUNDIALS spils SUNLINSOL implementations (SUNLINSOL_SPGMR, SUNLINSOL_SPFGMR, SUNLINSOL_SPBCGS, SUNLINSOL_SPTFQMR, or SUNLINSOL_PCG) as the outer solver. The creation and storage of the preconditioner matrix, and interfacing with the corresponding linear solver, can be handled through a package's preconditioner 'setup' and 'solve' functionality (see §4.5.8.2) without creating SUNMATRIX and SUNLINSOL implementations. This usage mode is recommended primarily because the SUNDIALS-provided spils modules support the scaling as described above.

A second approach supported by the linear solver APIs is as follows. If the SUNLINSOL implementation is matrix-based, *self-identifies as having* `SUNLINEARSOLVER_ITERATIVE` *type*, and *also provides a non-*`NULL` `SUNLinSolSetATimes` *routine*, then each SUNDIALS package will call that routine to attach its package-specific matrix-vector product routine to the SUNLINSOL object. The SUNDIALS package will then call the SUNLINSOL-provided `SUNLinSolSetup` routine (infrequently) to update matrix information, but will provide current matrix-vector products to the SUNLINSOL implementation through the package-supplied `ATimesFn` routine.

9.4 IDAS SUNLinearSolver interface

Table 9.3 below lists the SUNLINSOL module linear solver functions used within the IDALS interface. As with the SUNMATRIX module, we emphasize that the IDA user does not need to know detailed usage of linear solver functions by the IDA code modules in order to use IDA. The information is presented as an implementation detail for the interested reader.

The linear solver functions listed below are marked with ✓to indicate that they are required, or with † to indicate that they are only called if they are non-`NULL` in the SUNLINSOL implementation that is being used. Note:

1. Although IDALS does not call `SUNLinSolLastFlag` directly, this routine is available for users to query linear solver issues directly.

2. Although IDALS does not call `SUNLinSolFree` directly, this routine should be available for users to call when cleaning up from a simulation.

Table 9.3: List of linear solver function usage in the IDALS interface

	DIRECT	ITERATIVE	MATRIX_ITERATIVE
SUNLinSolGetType	✓	✓	✓
SUNLinSolSetATimes	†	✓	†
SUNLinSolSetPreconditioner	†	†	†
SUNLinSolSetScalingVectors	†	†	†
SUNLinSolInitialize	✓	✓	✓
SUNLinSolSetup	✓	✓	✓
SUNLinSolSolve	✓	✓	✓
SUNLinSolNumIters		✓	✓
SUNLinSolResid		✓	✓
[1]SUNLinSolLastFlag			
[2]SUNLinSolFree			
SUNLinSolSpace	†	†	†

Since there are a wide range of potential SUNLINSOL use cases, the following subsections describe some details of the IDALS interface, in the case that interested users wish to develop custom SUNLINSOL modules.

9.4.1 Lagged matrix information

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_DIRECT` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`, then the SUNLINSOL object solves a linear system *defined* by a SUNMATRIX object. CVLS will update the matrix information infrequently according to the strategies outlined in §2.1. When solving a linear system $J\bar{x} = b$, it is likely that the value $\bar{\alpha}$ used to construct J differs from the current value of α in the BDF method, since J is updated infrequently. Therefore, after calling the SUNLINSOL-provided `SUNLinSolSolve` routine, we test whether $\alpha/\bar{\alpha} \neq 1$, and if this is the case we scale the solution $\bar{x}$ to obtain the desired linear system solution x via

$$x = \frac{2}{1 + \alpha/\bar{\alpha}}\bar{x}. \tag{9.3}$$

For values of $\alpha/\bar{\alpha}$ that are "close" to 1, this rescaling approximately solves the original linear system.

9.4.2 Iterative linear solver tolerance

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE` then IDALS will set the input tolerance `delta` as described in §2.1. However, if the iterative linear solver does not support scaling matrices (i.e., the `SUNLinSolSetScalingVectors` routine is `NULL`), then IDALS will attempt to adjust the linear solver tolerance to account for this lack of functionality. To this end, the following assumptions are made:

1. All solution components have similar magnitude; hence the error weight vector W used in the WRMS norm (see §2.1) should satisfy the assumption

$$W_i \approx W_{mean}, \quad \text{for} \quad i = 0, \ldots, n-1.$$

2. The SUNLINSOL object uses a standard 2-norm to measure convergence.

Since IDA uses identical left and right scaling matrices, $S_1 = S_2 = S = \text{diag}(W)$, then the linear solver convergence requirement is converted as follows (using the notation from equations (9.1)-(9.2)):

$$\begin{aligned}
& \left\|\tilde{b} - \tilde{A}\tilde{x}\right\|_2 < \text{tol} \\
\Leftrightarrow \quad & \left\|SP_1^{-1}b - SP_1^{-1}Ax\right\|_2 < \text{tol} \\
\Leftrightarrow \quad & \sum_{i=0}^{n-1} \left[W_i \left(P_1^{-1}(b - Ax)\right)_i\right]^2 < \text{tol}^2 \\
\Leftrightarrow \quad & W_{mean}^2 \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax)\right)_i\right]^2 < \text{tol}^2 \\
\Leftrightarrow \quad & \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax)\right)_i\right]^2 < \left(\frac{\text{tol}}{W_{mean}}\right)^2 \\
\Leftrightarrow \quad & \left\|P_1^{-1}(b - Ax)\right\|_2 < \frac{\text{tol}}{W_{mean}}
\end{aligned}$$

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2/\sqrt{n}$$

is computed and the scaled tolerance `delta`$= \text{tol}/W_{mean}$ is supplied to the SUNLINSOL object.

9.5 The SUNLinearSolver_Dense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems. The SUNLINSOL_DENSE module 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).

To access the SUNLINSOL_DENSE module, include the header file `sunlinsol/sunlinsol_dense.h`. We note that the SUNLINSOL_DENSE module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsoldense` module library.

9.5.1 SUNLinearSolver_Dense description

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).

9.5.2 SUNLinearSolver_Dense functions

The SUNLINSOL_DENSE module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

SUNLinSol_Dense	
Call	`LS = SUNLinSol_Dense(y, A);`
Description	The function `SUNLinSol_Dense` creates and allocates memory for a dense `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	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.
Deprecated Name	For backward compatibility, the wrapper function `SUNDenseLinearSolver` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_Dense` when using the Fortran 2003 interface module.

The SUNLINSOL_DENSE module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

9.5.3 SUNLinearSolver_Dense Fortran interfaces

The SUNLINSOL_DENSE module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_dense_mod` FORTRAN module defines interfaces to all SUNLINSOL_DENSE C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_Dense` is interfaced as `FSUNLinSol_Dense`.

The FORTRAN 2003 SUNLINSOL_DENSE interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_dense_mod`, and linking to the library `libsundials_fsunlinsoldense_mod.`*lib* in

addition to the C library. For details on where the library and module file `fsunlinsol_dense_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsoldense_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_DENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNDENSELINSOLINIT`

Call `FSUNDENSELINSOLINIT(code, ier)`

Description The function `FSUNDENSELINSOLINIT` can be called for Fortran programs to create a dense `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes 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 SUNLINSOL_DENSE module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSDENSELINSOLINIT`

Call `FSUNMASSDENSELINSOLINIT(ier)`

Description The function `FSUNMASSDENSELINSOLINIT` can be called for Fortran programs to create a dense `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.5.4 SUNLinearSolver_Dense content

The SUNLINSOL_DENSE module defines the *content* field of a `SUNLinearSolver` as 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.

9.6 The SUNLinearSolver_Band implementation

This section describes the SUNLINSOL implementation for solving banded linear systems. The SUNLINSOL_BAND module 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).

To access the SUNLINSOL_BAND module, include the header file `sunlinsol/sunlinsol_band.h`. We note that the SUNLINSOL_BAND module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolband` module library.

9.6.1 SUNLinearSolver_Band description

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`.

9.6.2 SUNLinearSolver_Band functions

The SUNLINSOL_BAND module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_Band`

Call	`LS = SUNLinSol_Band(y, A);`
Description	The function `SUNLinSol_Band` creates and allocates memory for a band `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_BAND matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	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.
Deprecated Name	For backward compatibility, the wrapper function `SUNBandLinearSolver` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_Band` when using the Fortran 2003 interface module.

The SUNLINSOL_BAND module defines band implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

9.6.3 SUNLinearSolver_Band Fortran interfaces

The SUNLINSOL_BAND module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_band_mod` FORTRAN module defines interfaces to all SUNLINSOL_BAND C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_Band` is interfaced as `FSUNLinSol_Band`.

The FORTRAN 2003 SUNLINSOL_BAND interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_band_mod`, and linking to the library `libsundials_fsunlinsolband_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_band_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolband_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_BAND module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNBANDLINSOLINIT`

Call	`FSUNBANDLINSOLINIT(code, ier)`
Description	The function `FSUNBANDLINSOLINIT` can be called for Fortran programs to create a band `SUNLinearSolver` object.
Arguments	`code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
Return value	`ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.
Notes	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 SUNLINSOL_BAND module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

FSUNMASSBANDLINSOLINIT	
Call	`FSUNMASSBANDLINSOLINIT(ier)`
Description	The function `FSUNMASSBANDLINSOLINIT` can be called for Fortran programs to create a band `SUNLinearSolver` object for mass matrix linear systems.
Arguments	None
Return value	`ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.
Notes	This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.6.4 SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a `SUNLinearSolver` as 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.

9.7 The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LAPACK. The SUNLINSOL_LAPACKDENSE module 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).

To access the SUNLINSOL_LAPACKDENSE module, include the header file `sunlinsol/sunlinsol_lapackdense.h`. The installed module library to link to is `libsundials_sunlinsollapackdense.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

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 64-bit integers for the `sunindextype`.

9.7.1 SUNLinearSolver_LapackDense description

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).

9.7.2 SUNLinearSolver_LapackDense functions

The SUNLINSOL_LAPACKDENSE module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_LapackDense`

Call	`LS = SUNLinSol_LapackDense(y, A);`
Description	The function `SUNLinSol_LapackDense` creates and allocates memory for a LAPACK-based, dense `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	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.
Deprecated Name	For backward compatibility, the wrapper function `SUNLapackDense` with idential input and output arguments is also provided.

The SUNLINSOL_LAPACKDENSE module defines dense implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

9.7.3 SUNLinearSolver_LapackDense Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKDENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNLAPACKDENSEINIT`

Call `FSUNLAPACKDENSEINIT(code, ier)`

Description The function `FSUNLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based dense `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes 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 SUNLINSOL_LAPACKDENSE module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSLAPACKDENSEINIT`

Call `FSUNMASSLAPACKDENSEINIT(ier)`

Description The function `FSUNMASSLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based, dense `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.7.4 SUNLinearSolver_LapackDense content

The SUNLINSOL_LAPACKDENSE module defines the *content* field of a `SUNLinearSolver` as 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.

9.8 The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LAPACK. The SUNLINSOL_LAPACKBAND module 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).

To access the SUNLINSOL_LAPACKBAND module, include the header file `sunlinsol/sunlinsol_lapackband.h`. The installed module library to link to is `libsundials_sunlinsollapackband.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

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 64-bit integers for the sunindextype.

9.8.1 SUNLinearSolver_LapackBand description

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.

9.8.2 SUNLinearSolver_LapackBand functions

The SUNLINSOL_LAPACKBAND module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_LapackBand

Call	LS = SUNLinSol_LapackBand(y, A);
Description	The function SUNLinSol_LapackBand creates and allocates memory for a LAPACK-based, band SUNLinearSolver object.
Arguments	y (N_Vector) a template for cloning vectors needed within the solver A (SUNMatrix) a SUNMATRIX_BAND matrix template for cloning matrices needed within the solver
Return value	This returns a SUNLinearSolver object. If either A or y are incompatible then this routine will return NULL.
Notes	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.
Deprecated Name	For backward compatibility, the wrapper function SUNLapackBand with idential input and output arguments is also provided.

The SUNLINSOL_LAPACKBAND module defines band implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

9.8.3 SUNLinearSolver_LapackBand Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKBAND module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNLAPACKDENSEINIT`

Call `FSUNLAPACKBANDINIT(code, ier)`

Description The function `FSUNLAPACKBANDINIT` can be called for Fortran programs to create a LAPACK-based band `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes 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 SUNLINSOL_LAPACKBAND module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSLAPACKBANDINIT`

Call `FSUNMASSLAPACKBANDINIT(ier)`

Description The function `FSUNMASSLAPACKBANDINIT` can be called for Fortran programs to create a LAPACK-based, band `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.8.4 SUNLinearSolver_LapackBand content

The SUNLINSOL_LAPACKBAND module defines the *content* field of a `SUNLinearSolver` as 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.

9.9 The SUNLinearSolver_KLU implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with KLU. The SUNLINSOL_KLU module 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 header file to include when using this module is `sunlinsol/sunlinsol_klu.h`. The installed module library to link to is `libsundials_sunlinsolklu.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 17]. 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.

9.9.1 SUNLinearSolver_KLU description

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 or partial 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.

9.9.2 SUNLinearSolver_KLU functions

The SUNLINSOL_KLU module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_KLU`

Call	`LS = SUNLinSol_KLU(y, A);`
Description	The function `SUNLinSol_KLU` creates and allocates memory for a KLU-based `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	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.
Deprecated Name	For backward compatibility, the wrapper function `SUNKLU` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_KLU` when using the Fortran 2003 interface module.

The SUNLINSOL_KLU module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_KLU module also defines the following additional user-callable functions.

`SUNLinSol_KLUReInit`

Call `retval = SUNLinSol_KLUReInit(LS, A, nnz, reinit_type);`

Description The function `SUNLinSol_KLUReInit` 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).

Arguments

`LS`	(`SUNLinearSolver`) a template for cloning vectors needed within the solver
`A`	(`SUNMatrix`) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
`nnz`	(`sunindextype`) the new number of nonzeros in the matrix
`reinit_type`	(`int`) flag governing the level of reinitialization. The allowed values are:

- `SUNKLU_REINIT_FULL` – 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.
- `SUNKLU_REINIT_PARTIAL` – 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 `SUNLinSol_KLUReInit` call).

Return value 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`.

Notes 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.

This routine assumes no other changes to solver use are necessary.

Deprecated Name For backward compatibility, the wrapper function `SUNKLUReInit` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_KLUReInit` when using the Fortran 2003 interface module.

`SUNLinSol_KLUSetOrdering`

Call `retval = SUNLinSol_KLUSetOrdering(LS, ordering);`

Description This function sets the ordering used by KLU for reducing fill in the linear solve.

Arguments

`LS`	(`SUNLinearSolver`) the SUNLINSOL_KLU object
`ordering`	(`int`) flag indicating the reordering algorithm to use, the options are:

0 AMD,
1 COLAMD, and
2 the natural ordering.

The default is 1 for COLAMD.

Return value The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid ordering choice), or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNKLUSetOrdering` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_KLUSetOrdering` when using the Fortran 2003 interface module.

9.9.3 SUNLinearSolver_KLU Fortran interfaces

The SUNLINSOL_KLU module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_klu_mod` FORTRAN module defines interfaces to all SUNLINSOL_KLU C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_klu` is interfaced as `FSUNLinSol_klu`.

The FORTRAN 2003 SUNLINSOL_KLU interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_klu_mod`, and linking to the library `libsundials_fsunlinsolklu_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_klu_mod.mod` are installed see Appendix A.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_KLU module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNKLUINIT`

Call `FSUNKLUINIT(code, ier)`

Description The function `FSUNKLUINIT` can be called for Fortran programs to create a SUNLINSOL_KLU object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes 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 SUNLINSOL_KLU module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSKLUINIT`

Call `FSUNMASSKLUINIT(ier)`

Description The function `FSUNMASSKLUINIT` can be called for Fortran programs to create a KLU-based `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

The `SUNLinSol_KLUReInit` and `SUNLinSol_KLUSetOrdering` routines also support FORTRAN interfaces for the system and mass matrix solvers:

`FSUNKLUREINIT`

Call `FSUNKLUREINIT(code, nnz, reinit_type, ier)`

Description The function `FSUNKLUREINIT` can be called for Fortran programs to re-initialize a SUNLINSOL_KLU object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `nnz` (`sunindextype*`) the new number of nonzeros in the matrix
- `reinit_type` (`int*`) flag governing 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 `SUNLinSol_KLUReInit` call).

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUReInit` for complete further documentation of this routine.

`FSUNMASSKLUREINIT`

Call `FSUNMASSKLUREINIT(nnz, reinit_type, ier)`

Description The function `FSUNMASSKLUREINIT` can be called for Fortran programs to re-initialize a SUNLINSOL_KLU object for mass matrix linear systems.

Arguments The arguments are identical to `FSUNKLUREINIT` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUReInit` for complete further documentation of this routine.

`FSUNKLUSETORDERING`

Call `FSUNKLUSETORDERING(code, ordering, ier)`

Description The function `FSUNKLUSETORDERING` can be called for Fortran programs to change the reordering algorithm used by KLU.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `ordering` (`int*`) flag indication the reordering algorithm to use. Options include:
  - 0 AMD,
  - 1 COLAMD, and

2 the natural ordering.

The default is 1 for COLAMD.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUSetOrdering` for complete further documentation of this routine.

`FSUNMASSKLUSETORDERING`

Call `FSUNMASSKLUSETORDERING(ier)`

Description The function `FSUNMASSKLUSETORDERING` can be called for Fortran programs to change the reordering algorithm used by KLU for mass matrix linear systems.

Arguments The arguments are identical to `FSUNKLUSETORDERING` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUSetOrdering` for complete further documentation of this routine.

9.9.4 SUNLinearSolver_KLU content

The SUNLINSOL_KLU module defines the *content* field of a `SUNLinearSolver` as 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).

9.10 The SUNLinearSolver_SuperLUMT implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with SuperLU_MT. The SUPERLUMT module 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 header file to include when using this module is `sunlinsol/sunlinsol_superlumt.h`. The installed module library to link to is `libsundials_sunlinsolsuperlumt.`*`lib`* where `.`*`lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_SUPERLUMT module is a SUNLINSOL wrapper for the SUPERLUMT sparse matrix factorization and solver library written by X. Sherry Li [2, 35, 19]. 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.

9.10.1 SUNLinearSolver_SuperLUMT description

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.

9.10.2 SUNLinearSolver_SuperLUMT functions

The module SUNLINSOL_SUPERLUMT provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SuperLUMT`

Call	`LS = SUNLinSol_SuperLUMT(y, A, num_threads);`	
Description	The function `SUNLinSol_SuperLUMT` creates and allocates memory for a SuperLU_MT-based `SUNLinearSolver` object.	
Arguments	`y`	(`N_Vector`) a template for cloning vectors needed within the solver
	`A`	(`SUNMatrix`) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
	`num_threads`	(`int`) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.	

Notes 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.

The `num_threads` argument is not checked and is passed directly to SUPERLUMT routines.

Deprecated Name For backward compatibility, the wrapper function `SUNSuperLUMT` with idential input and output arguments is also provided.

The SUNLINSOL_SUPERLUMT module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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 SUNLINSOL_SUPERLUMT module also defines the following additional user-callable function.

`SUNLinSol_SuperLUMTSetOrdering`

Call `retval = SUNLinSol_SuperLUMTSetOrdering(LS, ordering);`

Description This function sets the ordering used by SUPERLUMT for reducing fill in the linear solve.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUMT object

`ordering` (`int`) a flag indicating the ordering algorithm to use, the options 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.

Return value The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid ordering choice), or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSuperLUMTSetOrdering` with idential input and output arguments is also provided.

9.10.3 SUNLinearSolver_SuperLUMT Fortran interfaces

For solvers that include a Fortran interface module, the SUNLINSOL_SUPERLUMT module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSUPERLUMTINIT`

Call `FSUNSUPERLUMTINIT(code, num_threads, ier)`

Description The function `FSUNSUPERLUMTINIT` can be called for Fortran programs to create a SUNLINSOL_KLU object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `num_threads` (`int*`) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes 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 SUNLINSOL_SUPERLUMT module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSUPERLUMTINIT`

Call `FSUNMASSSUPERLUMTINIT(num_threads, ier)`

Description The function `FSUNMASSSUPERLUMTINIT` can be called for Fortran programs to create a SuperLU_MT-based `SUNLinearSolver` object for mass matrix linear systems.

Arguments
- `num_threads` (`int*`) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

The `SUNLinSol_SuperLUMTSetOrdering` routine also supports Fortran interfaces for the system and mass matrix solvers:

`FSUNSUPERLUMTSETORDERING`

Call `FSUNSUPERLUMTSETORDERING(code, ordering, ier)`

Description The function `FSUNSUPERLUMTSETORDERING` can be called for Fortran programs to update the ordering algorithm in a SUNLINSOL_SUPERLUMT object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `ordering` (`int*`) a flag indicating the ordering algorithm, options 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.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SuperLUMTSetOrdering` for complete further documentation of this routine.

`FSUNMASSUPERLUMTSETORDERING`

Call `FSUNMASSUPERLUMTSETORDERING(ordering, ier)`

Description The function `FSUNMASSUPERLUMTSETORDERING` can be called for Fortran programs to update the ordering algorithm in a SUNLINSOL_SUPERLUMT object for mass matrix linear systems.

Arguments `ordering` (`int*`) a flag indicating the ordering algorithm, options 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.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SuperLUMTSetOrdering` for complete further documentation of this routine.

9.10.4 SUNLinearSolver_SuperLUMT content

The SUNLINSOL_SUPERLUMT module defines the *content* field of a `SUNLinearSolver` as 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.

9.11 The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [41]) iterative linear solver. The SUNLINSOL_SPGMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). When using Classical Gram-Schmidt, the optional function `N_VDotProdMulti` may be supplied for increased efficiency.

To access the SUNLINSOL_SPGMR module, include the header file `sunlinsol/sunlinsol_spgmr.h`. We note that the SUNLINSOL_SPGMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspgmr` module library.

9.11.1 SUNLinearSolver_SPGMR description

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.

9.11.2 SUNLinearSolver_SPGMR functions

The SUNLINSOL_SPGMR module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SPGMR`

Call: `LS = SUNLinSol_SPGMR(y, pretype, maxl);`

Description: The function `SUNLinSol_SPGMR` creates and allocates memory for a SPGMR `SUNLinearSolver` object.

Arguments:

- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values are:
  - `PREC_NONE` (0)
  - `PREC_LEFT` (1)
  - `PREC_RIGHT` (2)
  - `PREC_BOTH` (3)

  Any other integer input will result in the default (no preconditioning).
- `maxl` (`int`) the number of Krylov basis vectors to use. Values ≤ 0 will result in the default value (5).

Return value: This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.

Notes 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`.

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.

Deprecated Name For backward compatibility, the wrapper function `SUNSPGMR` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPGMR` when using the Fortran 2003 interface module.

The SUNLINSOL_SPGMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPGMR module also defines the following additional user-callable functions.

`SUNLinSol_SPGMRSetPrecType`

Call `retval = SUNLinSol_SPGMRSetPrecType(LS, pretype);`

Description The function `SUNLinSol_SPGMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPGMR object.

Arguments
- `LS` (`SUNLinearSolver`) the SUNLINSOL_SPGMR object to update
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPGMR`.

Return value This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSPGMRSetPrecType` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPGMRSetPrecType` when using the Fortran 2003 interface module.

`SUNLinSol_SPGMRSetGSType`

Call `retval = SUNLinSol_SPGMRSetGSType(LS, gstype);`

Description The function `SUNLinSol_SPGMRSetPrecType` sets the type of Gram-Schmidt orthogonalization to use in the SUNLINSOL_SPGMR object.

Arguments
- `LS` (`SUNLinearSolver`) the SUNLINSOL_SPGMR object to update
- `gstype` (`int`) flag indicating the desired orthogonalization algorithm; allowed values are:
  - `MODIFIED_GS` (1)
  - `CLASSICAL_GS` (2)

  Any other integer input will result in a failure, returning error code `SUNLS_ILL_INPUT`.

Return value This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSPGMRSetGSType` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPGMRSetGSType` when using the Fortran 2003 interface module.

`SUNLinSol_SPGMRSetMaxRestarts`

Call `retval = SUNLinSol_SPGMRSetMaxRestarts(LS, maxrs);`

Description The function `SUNLinSol_SPGMRSetMaxRestarts` sets the number of GMRES restarts to allow in the SUNLINSOL_SPGMR object.

Arguments
- `LS` (`SUNLinearSolver`) the SUNLINSOL_SPGMR object to update
- `maxrs` (`int`) integer indicating number of restarts to allow. A negative input will result in the default of 0.

Return value This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSPGMRSetMaxRestarts` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPGMRSetMaxRestarts` when using the Fortran 2003 interface module.

9.11.3 SUNLinearSolver_SPGMR Fortran interfaces

The SUNLINSOL_SPGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_spgmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPGMR` is interfaced as `FSUNLinSol_SPGMR`.

The FORTRAN 2003 SUNLINSOL_SPGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_spgmr_mod`, and linking to the library `libsundials_fsunlinsolspgmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_spgmr_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolspgmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPGMRINIT`

Call `FSUNSPGMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPGMRINIT`

Call `FSUNMASSSPGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

The `SUNLinSol_SPGMRSetPrecType`, `SUNLinSol_SPGMRSetGSType` and `SUNLinSol_SPGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPGMRSETGSTYPE`

Call `FSUNSPGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

FSUNMASSSPGMRSETGSTYPE

Call `FSUNMASSSPGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

FSUNSPGMRSETPRECTYPE

Call `FSUNSPGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

FSUNMASSSPGMRSETPRECTYPE

Call `FSUNMASSSPGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

FSUNSPGMRSETMAXRS

Call `FSUNSPGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

FSUNMASSSPGMRSETMAXRS

Call `FSUNMASSSPGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

9.11.4 SUNLinearSolver_SPGMR content

The SUNLINSOL_SPGMR module defines the *content* field of a `SUNLinearSolver` as 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.

9.12 The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [40]) iterative linear solver. The SUNLINSOL_SPFGMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). When using Classical Gram-Schmidt, the optional function `N_VDotProdMulti` may be supplied for increased efficiency. Unlike the other Krylov iterative linear solvers supplied with SUNDIALS, SPFGMR is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

To access the SUNLINSOL_SPFGMR module, include the header file `sunlinsol/sunlinsol_spfgmr.h`. We note that the SUNLINSOL_SPFGMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspfgmr` module library.

9.12.1 SUNLinearSolver_SPFGMR description

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.

9.12.2 SUNLinearSolver_SPFGMR functions

The SUNLINSOL_SPFGMR module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SPFGMR`

Call `LS = SUNLinSol_SPFGMR(y, pretype, maxl);`

Description The function `SUNLinSol_SPFGMR` creates and allocates memory for a SPFGMR `SUNLinearSolver` object.

Arguments
- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values are:
  - `PREC_NONE` (0)
  - `PREC_LEFT` (1)
  - `PREC_RIGHT` (2)
  - `PREC_BOTH` (3)

  Any other integer input will result in the default (no preconditioning).
- `maxl` (`int`) the number of Krylov basis vectors to use. Values ≤ 0 will result in the default value (5).

Return value This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.

Notes 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`.

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_SPFGMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

F2003 Name This function is callable as `FSUNLinSol_SPFGMR` when using the Fortran 2003 interface module.

SUNSPFGMR The SUNLINSOL_SPFGMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPFGMR module also defines the following additional user-callable functions.

SUNLinSol_SPFGMRSetPrecType

Call	`retval = SUNLinSol_SPFGMRSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPFGMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPFGMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPFGMR object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPFGMR`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPFGMRSetPrecType` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPFGMRSetPrecType` when using the Fortran 2003 interface module.

SUNLinSol_SPFGMRSetGSType

Call	`retval = SUNLinSol_SPFGMRSetGSType(LS, gstype);`
Description	The function `SUNLinSol_SPFGMRSetPrecType` sets the type of Gram-Schmidt orthogonalization to use in the SUNLINSOL_SPFGMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPFGMR object to update `gstype` (`int`) flag indicating the desired orthogonalization algorithm; allowed values are: • `MODIFIED_GS` (1) • `CLASSICAL_GS` (2) Any other integer input will result in a failure, returning error code `SUNLS_ILL_INPUT`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPFGMRSetGSType` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPFGMRSetGSType` when using the Fortran 2003 interface module.

`SUNLinSol_SPFGMRSetMaxRestarts`

Call	`retval = SUNLinSol_SPFGMRSetMaxRestarts(LS, maxrs);`
Description	The function `SUNLinSol_SPFGMRSetMaxRestarts` sets the number of GMRES restarts to allow in the SUNLINSOL_SPFGMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPFGMR object to update `maxrs` (`int`) integer indicating number of restarts to allow. A negative input will result in the default of 0.
Return value	This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPFGMRSetMaxRestarts` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPFGMRSetMaxRestarts` when using the Fortran 2003 interface module.

9.12.3 SUNLinearSolver_SPFGMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_spfgmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPFGMR` is interfaced as `FSUNLinSol_SPFGMR`.

The FORTRAN 2003 SUNLINSOL_SPFGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_spfgmr_mod`, and linking to the library `libsundials_fsunlinsolspfgmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_spfgmr_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolspfgmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPFGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPFGMRINIT`

Call	`FSUNSPFGMRINIT(code, pretype, maxl, ier)`
Description	The function `FSUNSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object.
Arguments	`code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE). `pretype` (`int*`) flag indicating desired preconditioning type `maxl` (`int*`) flag indicating Krylov subspace size
Return value	`ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.
Notes	This routine must be called *after* the NVECTOR object has been initialized. Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPFGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPFGMRINIT`

Call `FSUNMASSSPFGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object for mass matrix linear systems.

Arguments `pretype` (`int*`) flag indicating desired preconditioning type
`maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

The `SUNLinSol_SPFGMRSetPrecType`, `SUNLinSol_SPFGMRSetGSType` and `SUNLinSol_SPFGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPFGMRSETGSTYPE`

Call `FSUNSPFGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETGSTYPE`

Call `FSUNMASSSPFGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

`FSUNSPFGMRSETPRECTYPE`

Call `FSUNSPFGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETPRECTYPE`

Call `FSUNMASSSPFGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNSPFGMRSETMAXRS`

Call `FSUNSPFGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETMAXRS`

Call `FSUNMASSSPFGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

9.12.4 SUNLinearSolver_SPFGMR content

The SUNLINSOL_SPFGMR module defines the *content* field of a `SUNLinearSolver` as 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 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 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 (`maxl` + 1) × `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.

9.13 The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [44]) iterative linear solver. The SUNLINSOL_SPBCGS module is designed to be compatible with any NVECTOR implementation 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.

To access the SUNLINSOL_SPBCGS module, include the header file `sunlinsol/sunlinsol_spbcgs.h`. We note that the SUNLINSOL_SPBCGS module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspbcgs` module library.

9.13.1 SUNLinearSolver_SPBCGS description

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.

9.13.2 SUNLinearSolver_SPBCGS functions

The SUNLINSOL_SPBCGS module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SPBCGS`

Call `LS = SUNLinSol_SPBCGS(y, pretype, maxl);`

Description The function `SUNLinSol_SPBCGS` creates and allocates memory for a SPBCGS `SUNLinearSolver` object.

Arguments
- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values are:
  - `PREC_NONE` (0)

- PREC_LEFT (1)
- PREC_RIGHT (2)
- PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

`maxl` (`int`) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.

Notes 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`.

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.

Deprecated Name For backward compatibility, the wrapper function `SUNSPBCGS` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPBCGS` when using the Fortran 2003 interface module.

The SUNLINSOL_SPBCGS module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPBCGS module also defines the following additional user-callable functions.

`SUNLinSol_SPBCGSSetPrecType`

Call	`retval = SUNLinSol_SPBCGSSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPBCGSSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPBCGS object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPBCGS object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPBCGS`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPBCGSSetPrecType` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPBCGSSetPrecType` when using the Fortran 2003 interface module.

`SUNLinSol_SPBCGSSetMaxl`

Call	`retval = SUNLinSol_SPBCGSSetMaxl(LS, maxl);`
Description	The function `SUNLinSol_SPBCGSSetMaxl` updates the number of linear solver iterations to allow.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPBCGS object to update `maxl` (`int`) flag indicating the number of iterations to allow. Values ≤ 0 will result in the default value (5).
Return value	This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPBCGSSetMaxl` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPBCGSSetMaxl` when using the Fortran 2003 interface module.

9.13.3 SUNLinearSolver_SPBCGS Fortran interfaces

The SUNLINSOL_SPBCGS module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_spbcgs_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPBCGS C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPBCGS` is interfaced as `FSUNLinSol_SPBCGS`.

The FORTRAN 2003 SUNLINSOL_SPBCGS interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_spbcgs_mod`, and linking to the library `libsundials_fsunlinsolspbcgs_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_spbcgs_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolspbcgs_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPBCGS module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNSPBCGSINIT

Call `FSUNSPBCGSINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPBCGSINIT` can be called for Fortran programs to create a SUNLINSOL_SPBCGS object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPBCGS`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPBCGS module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

FSUNMASSSPBCGSINIT

Call `FSUNMASSSPBCGSINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPBCGSINIT` can be called for Fortran programs to create a SUNLINSOL_SPBCGS object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPBCGS`.

The `SUNLinSol_SPBCGSSetPrecType` and `SUNLinSol_SPBCGSSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPBCGSSETPRECTYPE

Call `FSUNSPBCGSSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPBCGSSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetPrecType` for complete further documentation of this routine.

FSUNMASSSPBCGSSETPRECTYPE

Call `FSUNMASSSPBCGSSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPBCGSSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPBCGSSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetPrecType` for complete further documentation of this routine.

`FSUNSPBCGSSETMAXL`

Call `FSUNSPBCGSSETMAXL(code, maxl, ier)`

Description The function `FSUNSPBCGSSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetMaxl` for complete further documentation of this routine.

`FSUNMASSSPBCGSSETMAXL`

Call `FSUNMASSSPBCGSSETMAXL(maxl, ier)`

Description The function `FSUNMASSSPBCGSSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPBCGSSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetMaxl` for complete further documentation of this routine.

9.13.4 SUNLinearSolver_SPBCGS content

The SUNLINSOL_SPBCGS module defines the *content* field of a `SUNLinearSolver` as 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.

9.14 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [23]) iterative linear solver. The SUNLINSOL_SPTFQMR module is designed to be compatible with any NVECTOR implementation 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.

To access the SUNLINSOL_SPTFQMR module, include the header file `sunlinsol/sunlinsol_sptfqmr.h`. We note that the SUNLINSOL_SPTFQMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolsptfqmr` module library.

9.14.1 SUNLinearSolver_SPTFQMR description

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.

9.14.2 SUNLinearSolver_SPTFQMR functions

The SUNLINSOL_SPTFQMR module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SPTFQMR`

Call `LS = SUNLinSol_SPTFQMR(y, pretype, maxl);`

Description The function `SUNLinSol_SPTFQMR` creates and allocates memory for a SPTFQMR `SUNLinearSolver` object.

Arguments
- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values are:
  - `PREC_NONE` (0)
  - `PREC_LEFT` (1)
  - `PREC_RIGHT` (2)
  - `PREC_BOTH` (3)

  Any other integer input will result in the default (no preconditioning).
- `maxl` (`int`) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.

Notes 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`.

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.

Deprecated Name For backward compatibility, the wrapper function `SUNSPTFQMR` with idential input and output arguments is also provided.

F2003 Name This function is callable as `FSUNLinSol_SPTFQMR` when using the Fortran 2003 interface module.

The SUNLINSOL_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPTFQMR module also defines the following additional user-callable functions.

`SUNLinSol_SPTFQMRSetPrecType`

Call	`retval = SUNLinSol_SPTFQMRSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPTFQMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPTFQMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPTFQMR object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPTFQMR`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPTFQMRSetPrecType` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_SPTFQMRSetPrecType` when using the Fortran 2003 interface module.

`SUNLinSol_SPTFQMRSetMaxl`

Call	`retval = SUNLinSol_SPTFQMRSetMaxl(LS, maxl);`
Description	The function `SUNLinSol_SPTFQMRSetMaxl` updates the number of linear solver iterations to allow.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPTFQMR object to update `maxl` (`int`) flag indicating the number of iterations to allow; values ≤ 0 will result in the default value (5)
Return value	This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
F2003 Name	This function is callable as `FSUNLinSol_SPTFQMRSetMaxl` when using the Fortran 2003 interface module.

SUNSPTFQMRSetMaxl

9.14.3 SUNLinearSolver_SPTFQMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_sptfqmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPTFQMR` is interfaced as `FSUNLinSol_SPTFQMR`.

The FORTRAN 2003 SUNLINSOL_SPFGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_sptfqmr_mod`, and linking to the library `libsundials_fsunlinsolsptfqmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_sptfqmr_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolsptfqmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPTFQMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPTFQMRINIT`

Call `FSUNSPTFQMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPTFQMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPTFQMRINIT`

Call `FSUNMASSSPTFQMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

The `SUNLinSol_SPTFQMRSetPrecType` and `SUNLinSol_SPTFQMRSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPTFQMRSETPRECTYPE`

Call `FSUNSPTFQMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPTFQMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPTFQMRSETPRECTYPE`

Call `FSUNMASSSPTFQMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPTFQMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPTFQMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetPrecType` for complete further documentation of this routine.

`FSUNSPTFQMRSETMAXL`

Call `FSUNSPTFQMRSETMAXL(code, maxl, ier)`

Description The function `FSUNSPTFQMRSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetMaxl` for complete further documentation of this routine.

`FSUNMASSSPTFQMRSETMAXL`

Call `FSUNMASSSPTFQMRSETMAXL(maxl, ier)`

Description The function `FSUNMASSSPTFQMRSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPTFQMRSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetMaxl` for complete further documentation of this routine.

9.14.4 SUNLinearSolver_SPTFQMR content

The SUNLINSOL_SPTFQMR module defines the *content* field of a `SUNLinearSolver` as 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.

9.15 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementaiton of the PCG (Preconditioned Conjugate Gradient [24]) iterative linear solver. The SUNLINSOL_PCG module is designed to be compatible with any NVECTOR implementation 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.

To access the SUNLINSOL_PCG module, include the header file `sunlinsol/sunlinsol_pcg.h`. We note that the SUNLINSOL_PCG module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolpcg` module library.

9.15.1 SUNLinearSolver_PCG description

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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.4}$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \tag{9.5}$$

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.

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.

9.15.2 SUNLinearSolver_PCG functions

The SUNLINSOL_PCG module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_PCG`

Call	`LS = SUNLinSol_PCG(y, pretype, maxl);`
Description	The function `SUNLinSol_PCG` creates and allocates memory for a PCG `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `pretype` (`int`) flag indicating whether to use preconditioning. 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). `maxl` (`int`) the number of linear iterations to allow; values ≤ 0 will result in the default value (5).
Return value	This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.
Notes	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`. 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.
Deprecated Name	For backward compatibility, the wrapper function `SUNPCG` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_PCG` when using the Fortran 2003 interface module.

The SUNLINSOL_PCG module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `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

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_PCG module also defines the following additional user-callable functions.

`SUNLinSol_PCGSetPrecType`

Call	`retval = SUNLinSol_PCGSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_PCGSetPrecType` updates the flag indicating use of preconditioning in the SUNLINSOL_PCG object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_PCG object to update `pretype` (`int`) flag indicating use of preconditioning, allowed values match those discussed in `SUNLinSol_PCG`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNPCGSetPrecType` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_PCGSetPrecType` when using the Fortran 2003 interface module.

`SUNLinSol_PCGSetMaxl`

Call	`retval = SUNLinSol_PCGSetMaxl(LS, maxl);`
Description	The function `SUNLinSol_PCGSetMaxl` updates the number of linear solver iterations to allow.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_PCG object to update `maxl` (`int`) flag indicating the number of iterations to allow; values ≤ 0 will result in the default value (5)
Return value	This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNPCGSetMaxl` with idential input and output arguments is also provided.
F2003 Name	This function is callable as `FSUNLinSol_PCGSetMaxl` when using the Fortran 2003 interface module.

9.15.3 SUNLinearSolver_PCG Fortran interfaces

The SUNLINSOL_PCG module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_pcg_mod` FORTRAN module defines interfaces to all SUNLINSOL_PCG C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_PCG` is interfaced as `FSUNLinSol_PCG`.

The FORTRAN 2003 SUNLINSOL_PCG interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_pcg_mod`, and linking to the library `libsundials_fsunlinsolpcg_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_pcg_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolpcg_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_PCG module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNPCGINIT`

Call `FSUNPCGINIT(code, pretype, maxl, ier)`

Description The function `FSUNPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_PCG module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSPCGINIT`

Call `FSUNMASSPCGINIT(pretype, maxl, ier)`

Description The function `FSUNMASSPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

The `SUNLinSol_PCGSetPrecType` and `SUNLinSol_PCGSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNPCGSETPRECTYPE`

Call `FSUNPCGSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNPCGSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetPrecType for complete further documentation of this routine.

FSUNMASSPCGSETPRECTYPE

Call FSUNMASSPCGSETPRECTYPE(pretype, ier)

Description The function FSUNMASSPCGSETPRECTYPE can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNPCGSETPRECTYPE above, except that code is not needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetPrecType for complete further documentation of this routine.

FSUNPCGSETMAXL

Call FSUNPCGSETMAXL(code, maxl, ier)

Description The function FSUNPCGSETMAXL can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

maxl (int*) the number of iterations to allow.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetMaxl for complete further documentation of this routine.

FSUNMASSPCGSETMAXL

Call FSUNMASSPCGSETMAXL(maxl, ier)

Description The function FSUNMASSPCGSETMAXL can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNPCGSETMAXL above, except that code is not needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_PCGSetMaxl for complete further documentation of this routine.

9.15.4 SUNLinearSolver_PCG content

The SUNLINSOL_PCG module defines the *content* field of a SUNLinearSolver as 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.

9.16 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.

Chapter 10

Description of the SUNNonlinearSolver module

SUNDIALS time integration packages are written in terms of generic nonlinear solver operations defined by the SUNNONLINSOL API and implemented by a particular SUNNONLINSOL module of type `SUNNonlinearSolver`. Users can supply their own SUNNONLINSOL module, or use one of the modules provided with SUNDIALS.

The time integrators in SUNDIALS specify a default nonlinear solver module and as such this chapter is intended for users that wish to use a non-default nonlinear solver module or would like to provide their own nonlinear solver implementation. Users interested in using a non-default solver module may skip the description of the SUNNONLINSOL API in section 10.1 and proceeded to the subsequent sections in this chapter that describe the SUNNONLINSOL modules provided with SUNDIALS.

For users interested in providing their own SUNNONLINSOL module, the following section presents the SUNNONLINSOL API and its implementation beginning with the definition of SUNNONLINSOL functions in sections 10.1.1 – 10.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 10.1.4. A table of nonlinear solver return codes is given in section 10.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 10.1.6. Section 10.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 10.1.8 lists the requirements for supplying a custom SUNNONLINSOL module. Users wishing to supply their own SUNNONLINSOL module are encouraged to use the SUNNONLINSOL implementations provided with SUNDIALS as a template for supplying custom nonlinear solver modules.

10.1 The SUNNonlinearSolver API

The SUNNONLINSOL API defines several nonlinear solver operations that enable SUNDIALS integrators to utilize any SUNNONLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core nonlinear solver functions. The second group of functions consists of set routines to supply the nonlinear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving nonlinear solver statistics. All of these functions are defined in the header file `sundials/sundials_nonlinearsolver.h`.

10.1.1 SUNNonlinearSolver core functions

The core nonlinear solver functions consist of two required functions to get the nonlinear solver type (`SUNNonlinsSolGetType`) and solve the nonlinear system (`SUNNonlinSolSolve`). The remaining three functions for nonlinear solver initialization (`SUNNonlinSolInitialization`), setup (`SUNNonlinSolSetup`), and destruction (`SUNNonlinSolFree`) are optional.

`SUNNonlinSolGetType`

Call `type = SUNNonlinSolGetType(NLS);`

Description The *required* function `SUNNonlinSolGetType` returns nonlinear solver type.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

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

`SUNNONLINEARSOLVER_ROOTFIND` 0, the SUNNONLINSOL module solves $F(y) = 0$.
`SUNNONLINEARSOLVER_FIXEDPOINT` 1, the SUNNONLINSOL module solves $G(y) = y$.

`SUNNonlinSolInitialize`

Call `retval = SUNNonlinSolInitialize(NLS);`

Description The *optional* function `SUNNonlinSolInitialize` performs nonlinear solver initialization and may perform any necessary memory allocations.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

Return value The return value `retval` (of type `int`) is zero for a successful call and a negative value for a failure.

Notes It is assumed all solver-specific options have been set prior to calling `SUNNonlinSolInitialize`. SUNNONLINSOL implementations that do not require initialization may set this operation to `NULL`.

`SUNNonlinSolSetup`

Call `retval = SUNNonlinSolSetup(NLS, y, mem);`

Description The *optional* function `SUNNonlinSolSetup` performs any solver setup needed for a nonlinear solve.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
`y` (`N_Vector`) the initial iteration passed to the nonlinear solver.
`mem` (`void *`) the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successful call and a negative value for a failure.

Notes SUNDIALS integrators call `SUNonlinSolSetup` before each step attempt. SUNNONLINSOL implementations that do not require setup may set this operation to `NULL`.

`SUNNonlinSolSolve`

Call `retval = SUNNonlinSolSolve(NLS, y0, y, w, tol, callLSetup, mem);`

Description The *required* function `SUNNonlinSolSolve` solves the nonlinear system $F(y) = 0$ or $G(y) = y$.

Arguments
`NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
`y0` (`N_Vector`) the initial iterate for the nonlinear solve. This *must* remain unchanged throughout the solution process.
`y` (`N_Vector`) the solution to the nonlinear system.
`w` (`N_Vector`) the solution error weight vector used for computing weighted error norms.
`tol` (`realtype`) the requested solution tolerance in the weighted root-mean-squared norm.
`callLSetup` (`booleantype`) a flag indicating that the integrator recommends for the linear solver setup function to be called.

`mem` (`void *`) the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

`SUNNonlinSolFree`

Call `retval = SUNNonlinSolFree(NLS);`

Description The *optional* function `SUNNonlinSolFree` frees any memory allocated by the nonlinear solver.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure. SUNNONLINSOL implementations that do not allocate data may set this operation to `NULL`.

10.1.2 SUNNonlinearSolver set functions

The following set functions are used to supply nonlinear solver modules with functions defined by the SUNDIALS integrators and to modify solver parameters. Only the routine for setting the nonlinear system defining function (`SUNNonlinSolSetSysFn` is required. All other set functions are optional.

`SUNNonlinSolSetSysFn`

Call `retval = SUNNonlinSolSetSysFn(NLS, SysFn);`

Description The *required* function `SUNNonlinSolSetSysFn` is used to provide the nonlinear solver with the function defining the nonlinear system. This is the function $F(y)$ in $F(y) = 0$ for `SUNNONLINEARSOLVER_ROOTFIND` modules or $G(y)$ in $G(y) = y$ for `SUNNONLINEARSOLVER_FIXEDPOINT` modules.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

`SysFn` (`SUNNonlinSolSysFn`) the function defining the nonlinear system. See section 10.1.4 for the definition of `SUNNonlinSolSysFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

`SUNNonlinSolSetLSetupFn`

Call `retval = SUNNonlinSolSetLSetupFn(NLS, LSetupFn);`

Description The *optional* function `SUNNonlinSolLSetupFn` is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver setup function.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

`LSetupFn` (`SUNNonlinSolLSetupFn`) a wrapper function to the SUNDIALS integrator's linear solver setup function. See section 10.1.4 for the definition of `SUNNonlinLSetupFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes The `SUNNonlinLSetupFn` function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLINSOL direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLINSOL iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize SUNLINSOL linear solvers, or use SUNLINSOL linear solvers that do not require setup may set this operation to `NULL`.

`SUNNonlinSolSetLSolveFn`

Call `retval = SUNNonlinSolSetLSolveFn(NLS, LSolveFn);`

Description The *optional* function `SUNNonlinSolSetLSolveFn` is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver solve function.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
- `LSolveFn` (`SUNNonlinSolLSolveFn`) a wrapper function to the SUNDIALS integrator's linear solver solve function. See section 10.1.4 for the definition of `SUNNonlinSolLSolveFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes The `SUNNonlinLSolveFn` function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNONLINSOL implementations that do not require solving this system or do not use SUNLINSOL linear solvers may set this operation to `NULL`.

`SUNNonlinSolSetConvTestFn`

Call `retval = SUNNonlinSolSetConvTestFn(NLS, CTestFn);`

Description The *optional* function `SUNNonlinSolSetConvTestFn` is used to provide the nonlinear solver with a function for determining if the nonlinear solver iteration has converged. This is typically called by SUNDIALS integrators to define their nonlinear convergence criteria, but may be replaced by the user.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
- `CTestFn` (`SUNNonlineSolConvTestFn`) a SUNDIALS integrator's nonlinear solver convergence test function. See section 10.1.4 for the definition of `SUNNonlinSolConvTestFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes SUNNONLINSOL implementations utilizing their own convergence test criteria may set this function to `NULL`.

`SUNNonlinSolSetMaxIters`

Call `retval = SUNNonlinSolSetMaxIters(NLS, maxiters);`

Description The *optional* function `SUNNonlinSolSetMaxIters` sets the maximum number of nonlinear solver iterations. This is typically called by SUNDIALS integrators to define their default iteration limit, but may be adjusted by the user.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
- `maxiters` (`int`) the maximum number of nonlinear iterations.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure (e.g., `maxiters` < 1).

10.1.3 SUNNonlinearSolver get functions

The following get functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routines to get the current total number of iterations (`SUNNonlinSolGetNumIters`) and number of convergence failures (`SUNNonlinSolGetNumConvFails`) are optional. The routine to get the current nonlinear solver iteration (`SUNNonlinSolGetCurIter`) is required when using the convergence test provided by the SUNDIALS integrator or by the ARKODE and CVODE linear solver interfaces. Otherwise, `SUNNonlinSolGetCurIter` is optional.

`SUNNonlinSolGetNumIters`

Call `retval = SUNNonlinSolGetNumIters(NLS, numiters);`

Description The *optional* function `SUNNonlinSolGetNumIters` returns the total number of nonlinear solver iterations. This is typically called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`numiters` (`long int*`) the total number of nonlinear solver iterations.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

`SUNNonlinSolGetCurIter`

Call `retval = SUNNonlinSolGetCurIter(NLS, iter);`

Description The function `SUNNonlinSolGetCurIter` returns the iteration index of the current nonlinear solve. This function is *required* when using SUNDIALS integrator-provided convergence tests or when using a SUNLINSOL spils linear solver; otherwise it is *optional*.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`iter` (`int*`) the nonlinear solver iteration in the current solve starting from zero.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

`SUNNonlinSolGetNumConvFails`

Call `retval = SUNNonlinSolGetNumConvFails(NLS, nconvfails);`

Description The *optional* function `SUNNonlinSolGetNumConvFails` returns the total number of nonlinear solver convergence failures. This may be called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`nconvfails` (`long int*`) the total number of nonlinear solver convergence failures.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

10.1.4 Functions provided by SUNDIALS integrators

To interface with SUNNONLINSOL modules, the SUNDIALS integrators supply a variety of routines for evaluating the nonlinear system, calling the SUNLINSOL setup and solve functions, and testing the nonlinear iteration for convergence. These integrator-provided routines translate between the user-supplied ODE or DAE systems and the generic interfaces to the nonlinear or linear systems of equations that result in their solution. The types for functions provided to a SUNNONLINSOL module are defined in the header file `sundials/sundials_nonlinearsolver.h`, and are described below.

`SUNNonlinSolSysFn`

Definition `typedef int (*SUNNonlinSolSysFn)(N_Vector y, N_Vector F, void* mem);`

Purpose These functions evaluate the nonlinear system $F(y)$ for `SUNNONLINEARSOLVER_ROOTFIND` type modules or $G(y)$ for `SUNNONLINEARSOLVER_FIXEDPOINT` type modules. Memory for `F` must by be allocated prior to calling this function. The vector `y` *must* be left unchanged.

Arguments `y` is the state vector at which the nonlinear system should be evaluated.
`F` is the output vector containing $F(y)$ or $G(y)$, depending on the solver type.

`mem` is the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

`SUNNonlinSolLSetupFn`

Definition
```
typedef int (*SUNNonlinSolLSetupFn)(N_Vector y, N_Vector F,
                                    booleantype jbad,
                                    booleantype* jcur, void* mem);
```

Purpose These functions are wrappers to the SUNDIALS integrator's function for setting up linear solves with SUNLINSOL modules.

Arguments
- `y` is the state vector at which the linear system should be setup.
- `F` is the value of the nonlinear system function at `y`.
- `jbad` is an input indicating whether the nonlinear solver believes that A has gone stale (`SUNTRUE`) or not (`SUNFALSE`).
- `jcur` is an output indicating whether the routine has updated the Jacobian A (`SUNTRUE`) or not (`SUNFALSE`).
- `mem` is the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

Notes The `SUNNonlinLSetupFn` function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLINSOL direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLINSOL iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize SUNLINSOL linear solvers, or use SUNLINSOL linear solvers that do not require setup may ignore these functions.

`SUNNonlinSolLSolveFn`

Definition
```
typedef int (*SUNNonlinSolLSolveFn)(N_Vector y, N_Vector b, void* mem);
```

Purpose These functions are wrappers to the SUNDIALS integrator's function for solving linear systems with SUNLINSOL modules.

Arguments
- `y` is the input vector containing the current nonlinear iteration.
- `b` contains the right-hand side vector for the linear solve on input and the solution to the linear system on output.
- `mem` is the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

Notes The `SUNNonlinLSolveFn` function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNONLINSOL implementations that do not require solving this system or do not use SUNLINSOL linear solvers may ignore these functions.

`SUNNonlinSolConvTestFn`

Definition
```
typedef int (*SUNNonlinSolConvTestFn)(SUNNonlinearSolver NLS, N_Vector y,
                                      N_Vector del, realtype tol,
                                      N_Vector ewt, void* mem);
```

Purpose These functions are SUNDIALS integrator-specific convergence tests for nonlinear solvers and are typically supplied by each SUNDIALS integrator, but users may supply custom problem-specific versions as desired.

Arguments
- `NLS` is the SUNNONLINSOL object.
- `y` is the current nonlinear iterate.
- `del` is the difference between the current and prior nonlinear iterates.
- `tol` is the nonlinear solver tolerance.
- `ewt` is the weight vector used in computing weighted norms.
- `mem` is the SUNDIALS integrator memory structure.

Return value The return value of this routine will be a negative value if an unrecoverable error occurred or one of the following:
- `SUN_NLS_SUCCESS` the iteration is converged.
- `SUN_NLS_CONTINUE` the iteration has not converged, keep iterating.
- `SUN_NLS_CONV_RECVR` the iteration appears to be diverging, try to recover.

Notes The tolerance passed to this routine by SUNDIALS integrators is the tolerance in a weighted root-mean-squared norm with error weight vector `ewt`. SUNNONLINSOL modules utilizing their own convergence criteria may ignore these functions.

10.1.5 SUNNonlinearSolver return codes

The functions provided to SUNNONLINSOL modules by each SUNDIALS integrator, and functions within the SUNDIALS-provided SUNNONLINSOL implementations utilize a common set of return codes, shown below in Table 10.1. Here, negative values correspond to non-recoverable failures, positive values to recoverable failures, and zero to a successful call.

Table 10.1: Description of the `SUNNonlinearSolver` return codes

Name	Value	Description
`SUN_NLS_SUCCESS`	`0`	successful call or converged solve
`SUN_NLS_CONTINUE`	`1`	the nonlinear solver is not converged, keep iterating
`SUN_NLS_CONV_RECVR`	`2`	the nonlinear solver appears to be diverging, try to recover
`SUN_NLS_MEM_NULL`	`-1`	a memory argument is `NULL`
`SUN_NLS_MEM_FAIL`	`-2`	a memory access or allocation failed
`SUN_NLS_ILL_INPUT`	`-3`	an illegal input option was provided

10.1.6 The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic SUNNONLINSOL module on which all other SUNNONLINSOL implementations are built. The `SUNNonlinearSolver` type is a pointer to a structure containing an implementation-dependent *content* field and an *ops* field. The type `SUNNonlinearSolver` is defined as follows:

```
typedef struct _generic_SUNNonlinearSolver *SUNNonlinearSolver;

struct _generic_SUNNonlinearSolver {
  void *content;
  struct _generic_SUNNonlinearSolver_Ops *ops;
};
```

where the `_generic_SUNNonlinearSolver_Ops` structure is a list of pointers to the various actual nonlinear solver operations provided by a specific implementation. The `_generic_SUNNonlinearSolver_Ops` structure is defined as

```
struct _generic_SUNNonlinearSolver_Ops {
  SUNNonlinearSolver_Type (*gettype)(SUNNonlinearSolver);
  int                     (*initialize)(SUNNonlinearSolver);
  int                     (*setup)(SUNNonlinearSolver, N_Vector, void*);
  int                     (*solve)(SUNNonlinearSolver, N_Vector, N_Vector,
                                   N_Vector, realtype, booleantype, void*);
  int                     (*free)(SUNNonlinearSolver);
  int                     (*setsysfn)(SUNNonlinearSolver, SUNNonlinSolSysFn);
  int                     (*setlsetupfn)(SUNNonlinearSolver, SUNNonlinSolLSetupFn);
  int                     (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
  int                     (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn);
  int                     (*setmaxiters)(SUNNonlinearSolver, int);
  int                     (*getnumiters)(SUNNonlinearSolver, long int*);
  int                     (*getcuriter)(SUNNonlinearSolver, int*);
  int                     (*getnumconvfails)(SUNNonlinearSolver, long int*);
};
```

The generic SUNNONLINSOL module defines and implements the nonlinear solver operations defined in Sections 10.1.1 – 10.1.3. These routines are in fact only wrappers to the nonlinear solver operations provided by a particular SUNNONLINSOL implementation, which are accessed through the ops field of the `SUNNonlinearSolver` structure. To illustrate this point we show below the implementation of a typical nonlinear solver operation from the generic SUNNONLINSOL module, namely `SUNNonlinSolSolve`, which solves the nonlinear system and returns a flag denoting a successful or failed solve:

```
int SUNNonlinSolSolve(SUNNonlinearSolver NLS,
                      N_Vector y0, N_Vector y,
                      N_Vector w, realtype tol,
                      booleantype callLSetup, void* mem)
{
  return((int) NLS->ops->solve(NLS, y0, y, w, tol, callLSetup, mem));
}
```

10.1.7 Usage with sensitivity enabled integrators

When used with SUNDIALS packages that support sensitivity analysis capabilities (e.g., CVODES and IDAS) a special NVECTOR module is used to interface with SUNNONLINSOL modules for solves involving sensitivity vectors stored in an NVECTOR array. As described below, the NVECTOR_SENSWRAPPER module is an NVECTOR implementation where the vector content is an NVECTOR array. This wrapper vector allows SUNNONLINSOL modules to operate on data stored as a collection of vectors.

For all SUNDIALS-provided SUNNONLINSOL modules a special constructor wrapper is provided so users do not need to interact directly with the NVECTOR_SENSWRAPPER module. These constructors follow the naming convention `SUNNonlinSol_***Sens(count,...)` where `***` is the name of the SUNNONLINSOL module, `count` is the size of the vector wrapper, and `...` are the module-specific constructor arguments.

The NVECTOR_SENSWRAPPER module

This section describes the NVECTOR_SENSWRAPPER implementation of an NVECTOR. To access the NVECTOR_SENSWRAPPER module, include the header file
`sundials/sundials_nvector_senswrapper.h`.

The NVECTOR_SENSWRAPPER module defines an `N_Vector` implementing all of the standard vectors operations defined in Table 7.2 but with some changes to how operations are computed in order to accommodate operating on a collection of vectors.

1. Element-wise vector operations are computed on a vector-by-vector basis. For example, the linear sum of two wrappers containing n_v vectors of length n, `N_VLinearSum(a,x,b,y,z)`, is computed as
$$z_{j,i} = ax_{j,i} + by_{j,i}, \quad i = 0, \ldots, n-1, \quad j = 0, \ldots, n_v - 1.$$

2. The dot product of two wrappers containing n_v vectors of length n is computed as if it were the dot product of two vectors of length nn_v. Thus `d = N_VDotProd(x,y)` is
$$d = \sum_{j=0}^{n_v-1} \sum_{i=0}^{n-1} x_{j,i} y_{j,i}.$$

3. All norms are computed as the maximum of the individual norms of the n_v vectors in the wrapper. For example, the weighted root mean square norm `m = N_VWrmsNorm(x, w)` is
$$m = \max_j \sqrt{\left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i})^2\right)}$$

To enable usage alongside other NVECTOR modules the NVECTOR_SENSWRAPPER functions implementing vector operations have `_SensWrapper` appended to the generic vector operation name.

The NVECTOR_SENSWRAPPER module provides the following constructors for creating an NVECTOR_SENSWRAPPER:

`N_VNewEmpty_SensWrapper`

Call `w = N_VNewEmpty_SensWrapper(count);`

Description The function `N_VNewEmpty_SensWrapper` creates an empty NVECTOR_SENSWRAPPER wrapper with space for `count` vectors.

Arguments `count` (`int`) the number of vectors the wrapper will contain.

Return value The return value `w` (of type `N_Vector`) will be a NVECTOR object if the constructor exits successfully, otherwise `w` will be `NULL`.

`N_VNew_SensWrapper`

Call `w = N_VNew_SensWrapper(count, y);`

Description The function `N_VNew_SensWrapper` creates an NVECTOR_SENSWRAPPER wrapper containing `count` vectors cloned from `y`.

Arguments `count` (`int`) the number of vectors the wrapper will contain.
`y` (`N_Vector`) the template vectors to use in creating the vector wrapper.

Return value The return value `w` (of type `N_Vector`) will be a NVECTOR object if the constructor exits successfully, otherwise `w` will be `NULL`.

The NVECTOR_SENSWRAPPER implementation of the NVECTOR module defines the *content* field of the `N_Vector` to be a structure containing an `N_Vector` array, the number of vectors in the vector array, and a boolean flag indicating ownership of the vectors in the vector array.

```
struct _N_VectorContent_SensWrapper {
  N_Vector* vecs;
  int nvecs;
  booleantype own_vecs;
};
```

The following macros are provided to access the content of an NVECTOR_SENSWRAPPER vector.

- `NV_CONTENT_SW(v)` - provides access to the content structure
- `NV_VECS_SW(v)` - provides access to the vector array
- `NV_NVECS_SW(v)` - provides access to the number of vectors
- `NV_OWN_VECS_SW(v)` - provides access to the ownership flag
- `NV_VEC_SW(v,i)` - provides access to the `i`-th vector in the vector array

10.1.8 Implementing a Custom SUNNonlinearSolver Module

A SUNNONLINSOL implementation *must* do the following:

1. Specify the content of the SUNNONLINSOL module.
2. Define and implement the required nonlinear solver operations defined in Sections 10.1.1 – 10.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one SUNNONLINSOL module (each with different `SUNNonlinearSolver` internal data representations) in the same code.
3. Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

1. Define and implement additional user-callable "set" routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.
2. Provide additional user-callable "get" routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

10.2 The SUNNonlinearSolver_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton's method. To access the SUNNONLINSOL_NEWTON module, include the header file `sunnonlinsol/sunnonlinsol_newton.h`. We note that the SUNNONLINSOL_NEWTON module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolnewton` module library.

10.2.1 SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{10.1}$$

given an initial guess $y^{(0)}$, Newton's method computes a series of approximate solutions

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{10.2}$$

where m is the Newton iteration index, and the Newton update $\delta^{(m+1)}$ is the solution of the linear system

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)})\,, \tag{10.3}$$

in which A is the Jacobian matrix

$$A \equiv \partial F/\partial y\,. \tag{10.4}$$

Depending on the linear solver used, the SUNNONLINSOL_NEWTON module will employ either a Modified Newton method, or an Inexact Newton method [5, 9, 18, 20, 33]. When used with a direct linear solver, the Jacobian matrix A is held constant during the Newton iteration, resulting in a Modified Newton method. With a matrix-free iterative linear solver, the iteration is an Inexact Newton method.

In both cases, calls to the integrator-supplied SUNNonlinSolLSetupFn function are made infrequently to amortize the increased cost of matrix operations (updating A and its factorization within direct linear solvers, or updating the preconditioner within iterative linear solvers). Specifically, SUNNONLINSOL_NEWTON will call the SUNNonlinSolLSetupFn function in two instances:

(a) when requested by the integrator (the input callLSetSetup is SUNTRUE) before attempting the Newton iteration, or

(b) when reattempting the nonlinear solve after a recoverable failure occurs in the Newton iteration with stale Jacobian information (jcur is SUNFALSE). In this case, SUNNONLINSOL_NEWTON will set jbad to SUNTRUE before calling the SUNNonlinSolLSetupFn function.

Whether the Jacobian matrix A is fully or partially updated depends on logic unique to each integrator-supplied SUNNonlinSolSetupFn routine. We refer to the discussion of nonlinear solver strategies provided in Chapter 2 for details on this decision.

The default maximum number of iterations and the stopping criteria for the Newton iteration are supplied by the SUNDIALS integrator when SUNNONLINSOL_NEWTON is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling the SUNNonlinSolSetMaxIters and/or SUNNonlinSolSetConvTestFn functions after attaching the SUNNONLINSOL_NEWTON object to the integrator.

10.2.2 SUNNonlinearSolver_Newton functions

The SUNNONLINSOL_NEWTON module provides the following constructors for creating a SUNNonlinearSolver object.

SUNNonlinSol_Newton

Call `NLS = SUNNonlinSol_Newton(y);`

Description The function SUNNonlinSol_Newton creates a SUNNonlinearSolver object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ using Newton's method.

Arguments `y` (N_Vector) a template for cloning vectors needed within the solver.

Return value The return value NLS (of type SUNNonlinearSolver) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise NLS will be NULL.

F2003 Name This function is callable as FSUNNonlinSol_Newton when using the Fortran 2003 interface module.

SUNNonlinSol_NewtonSens

Call `NLS = SUNNonlinSol_NewtonSens(count, y);`

Description The function SUNNonlinSol_NewtonSens creates a SUNNonlinearSolver object for use with SUNDIALS sensitivity enabled integrators (CVODES and IDAS) to solve nonlinear systems of the form $F(y) = 0$ using Newton's method.

Arguments `count` (int) the number of vectors in the nonlinear solve. When integrating a system containing Ns sensitivities the value of count is:

- Ns+1 if using a *simultaneous* corrector approach.
- Ns if using a *staggered* corrector approach.

`y` (N_Vector) a template for cloning vectors needed within the solver.

Return value The return value NLS (of type SUNNonlinearSolver) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise NLS will be NULL.

F2003 Name This function is callable as FSUNNonlinSol_NewtonSens when using the Fortran 2003 interface module.

The SUNNONLINSOL_NEWTON module implements all of the functions defined in sections 10.1.1 – 10.1.3 except for the `SUNNonlinSolSetup` function. The SUNNONLINSOL_NEWTON functions have the same names as those defined by the generic SUNNONLINSOL API with `_Newton` appended to the function name. Unless using the SUNNONLINSOL_NEWTON module as a standalone nonlinear solver the generic functions defined in sections 10.1.1 – 10.1.3 should be called in favor of the SUNNONLINSOL_NEWTON-specific implementations.

The SUNNONLINSOL_NEWTON module also defines the following additional user-callable function.

`SUNNonlinSolGetSysFn_Newton`

Call `retval = SUNNonlinSolGetSysFn_Newton(NLS, SysFn);`

Description The function `SUNNonlinSolGetSysFn_Newton` returns the residual function that defines the nonlinear system.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`SysFn` (`SUNNonlinSolSysFn*`) the function defining the nonlinear system.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes This function is intended for users that wish to evaluate the nonlinear residual in a custom convergence test function for the SUNNONLINSOL_NEWTON module. We note that SUNNONLINSOL_NEWTON will not leverage the results from any user calls to `SysFn`.

F2003 Name This function is callable as `FSUNNonlinSolGetSysFn_Newton` when using the Fortran 2003 interface module.

10.2.3 SUNNonlinearSolver_Newton Fortran interfaces

The SUNNONLINSOL_NEWTON module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunnonlinsol_newton_mod` FORTRAN module defines interfaces to all SUNNONLINSOL_NEWTON C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNNonlinSol_Newton` is interfaced as `FSUNNonlinSol_Newton`.

The FORTRAN 2003 SUNNONLINSOL_NEWTON interface module can be accessed with the `use` statement, i.e. `use fsunnonlinsol_newton_mod`, and linking to the library `libsundials_fsunnonlinsolnewton_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunnonlinsol_newton_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunnonlinsolnewton_mod` library.

FORTRAN 77 interface functions

For SUNDIALS integrators that include a FORTRAN 77 interface, the SUNNONLINSOL_NEWTON module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

`FSUNNEWTONINIT`

Call `FSUNNEWTONINIT(code, ier);`

Description The function `FSUNNEWTONINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ with Newton's method.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

10.2.4 SUNNonlinearSolver_Newton content

The SUNNONLINSOL_NEWTON module defines the *content* field of a `SUNNonlinearSolver` as the following structure:

```
struct _SUNNonlinearSolverContent_Newton {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolLSetupFn   LSetup;
  SUNNonlinSolLSolveFn   LSolve;
  SUNNonlinSolConvTestFn CTest;

  N_Vector    delta;
  booleantype jcur;
  int         curiter;
  int         maxiters;
  long int    niters;
  long int    nconvfails;
};
```

These entries of the *content* field contain the following information:

`Sys` - the function for evaluating the nonlinear system,

`LSetup` - the package-supplied function for setting up the linear solver,

`LSolve` - the package-supplied function for performing a linear solve,

`CTest` - the function for checking convergence of the Newton iteration,

`delta` - the Newton iteration update vector,

`jcur` - the Jacobian status (`SUNTRUE` = current, `SUNFALSE` = stale),

`curiter` - the current number of iterations in the solve attempt,

`maxiters` - the maximum number of Newton iterations allowed in a solve, and

`niters` - the total number of nonlinear iterations across all solves.

`nconvfails` - the total number of nonlinear convergence failures across all solves.

10.3 The SUNNonlinearSolver_FixedPoint implementation

This section describes the SUNNONLINSOL implementation of a fixed point (functional) iteration with optional Anderson acceleration. To access the SUNNONLINSOL_FIXEDPOINT module, include the header file `sunnonlinsol/sunnonlinsol_fixedpoint.h`. We note that the SUNNONLINSOL_FIXEDPOINT module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolfixedpoint` module library.

10.3.1 SUNNonlinearSolver_FixedPoint description

To find the solution to

$$G(y) = y \tag{10.5}$$

given an initial guess $y^{(0)}$, the fixed point iteration computes a series of approximate solutions

$$y^{(n+1)} = G(y^{(n)}) \tag{10.6}$$

where n is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [3, 45, 21, 36]. With Anderson acceleration using subspace size m, the series of approximate solutions can be formulated as the linear combination

$$y^{(n+1)} = \sum_{i=0}^{m_n} \alpha_i^{(n)} G(y^{(n-m_n+i)}) \tag{10.7}$$

where $m_n = \min\{m, n\}$ and the factors

$$\alpha^{(n)} = (\alpha_0^{(n)}, \ldots, \alpha_{m_n}^{(n)}) \tag{10.8}$$

solve the minimization problem $\min_\alpha \|F_n \alpha^T\|_2$ under the constraint that $\sum_{i=0}^{m_n} \alpha_i = 1$ where

$$F_n = (f_{n-m_n}, \ldots, f_n) \tag{10.9}$$

with $f_i = G(y^{(i)}) - y^{(i)}$. Due to this constraint, in the limit of $m = 0$ the accelerated fixed point iteration formula (10.7) simplifies to the standard fixed point iteration (10.6).

Following the recommendations made in [45], the SUNNONLINSOL_FIXEDPOINT implementation computes the series of approximate solutions as

$$y^{(n+1)} = G(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} \tag{10.10}$$

with $\Delta g_i = G(y^{(i+1)}) - G(y^{(i)})$ and where the factors

$$\gamma^{(n)} = (\gamma_0^{(n)}, \ldots, \gamma_{m_n-1}^{(n)}) \tag{10.11}$$

solve the unconstrained minimization problem $\min_\gamma \|f_n - \Delta F_n \gamma^T\|_2$ where

$$\Delta F_n = (\Delta f_{n-m_n}, \ldots, \Delta f_{n-1}), \tag{10.12}$$

with $\Delta f_i = f_{i+1} - f_i$. The least-squares problem is solved by applying a QR factorization to $\Delta F_n = Q_n R_n$ and solving $R_n \gamma = Q_n^T f_n$.

The acceleration subspace size m is required when constructing the SUNNONLINSOL_FIXEDPOINT object. The default maximum number of iterations and the stopping criteria for the fixed point iteration are supplied by the SUNDIALS integrator when SUNNONLINSOL_FIXEDPOINT is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling `SUNNonlinSolSetMaxIters` and `SUNNonlinSolSetConvTestFn` functions after attaching the SUNNONLINSOL_FIXEDPOINT object to the integrator.

10.3.2 SUNNonlinearSolver_FixedPoint functions

The SUNNONLINSOL_FIXEDPOINT module provides the following constructors for creating a `SUNNonlinearSolver` object.

`SUNNonlinSol_FixedPoint`

Call	`NLS = SUNNonlinSol_FixedPoint(y, m);`
Description	The function `SUNNonlinSol_FixedPoint` creates a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `m` (`int`) the number of acceleration vectors to use
Return value	The return value `NLS` (of type `SUNNonlinearSolver`) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise `NLS` will be `NULL`.
F2003 Name	This function is callable as `FSUNNonlinSol_FixedPoint` when using the Fortran 2003 interface module.

`SUNNonlinSol_FixedPointSens`

Call `NLS = SUNNonlinSol_FixedPointSens(count, y, m);`

Description The function `SUNNonlinSol_FixedPointSens` creates a `SUNNonlinearSolver` object for use with SUNDIALS sensitivity enabled integrators (CVODES and IDAS) to solve nonlinear systems of the form $G(y) = y$.

Arguments `count` (`int`) the number of vectors in the nonlinear solve. When integrating a system containing `Ns` sensitivities the value of `count` is:

- `Ns+1` if using a *simultaneous* corrector approach.
- `Ns` if using a *staggered* corrector approach.

`y` (`N_Vector`) a template for cloning vectors needed within the solver.

`m` (`int`) the number of acceleration vectors to use.

Return value The return value `NLS` (of type `SUNNonlinearSolver`) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise `NLS` will be `NULL`.

F2003 Name This function is callable as `FSUNNonlinSol_FixedPointSens` when using the Fortran 2003 interface module.

Since the accelerated fixed point iteration (10.6) does not require the setup or solution of any linear systems, the SUNNONLINSOL_FIXEDPOINT module implements all of the functions defined in sections 10.1.1 – 10.1.3 except for the `SUNNonlinSolSetup`, `SUNNonlinSolSetLSetupFn`, and `SUNNonlinSolSetLSolveFn` functions, that are set to `NULL`. The SUNNONLINSOL_FIXEDPOINT functions have the same names as those defined by the generic SUNNONLINSOL API with `_FixedPoint` appended to the function name. Unless using the SUNNONLINSOL_FIXEDPOINT module as a standalone nonlinear solver the generic functions defined in sections 10.1.1 – 10.1.3 should be called in favor of the SUNNONLINSOL_FIXEDPOINT-specific implementations.

The SUNNONLINSOL_FIXEDPOINT module also defines the following additional user-callable function.

`SUNNonlinSolGetSysFn_FixedPoint`

Call `retval = SUNNonlinSolGetSysFn_FixedPoint(NLS, SysFn);`

Description The function `SUNNonlinSolGetSysFn_FixedPoint` returns the fixed-point function that defines the nonlinear system.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object

`SysFn` (`SUNNonlinSolSysFn*`) the function defining the nonlinear system.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes This function is intended for users that wish to evaluate the fixed-point function in a custom convergence test function for the SUNNONLINSOL_FIXEDPOINT module. We note that SUNNONLINSOL_FIXEDPOINT will not leverage the results from any user calls to `SysFn`.

F2003 Name This function is callable as `FSUNNonlinSolGetSysFn_FixedPoint` when using the Fortran 2003 interface module.

10.3.3 SUNNonlinearSolver_FixedPoint Fortran interfaces

The SUNNONLINSOL_FIXEDPOINT module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunnonlinsol_fixedpoint_mod` FORTRAN module defines interfaces to all SUNNONLINSOL_FIXEDPOINT C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNNonlinSol_FixedPoint` is interfaced as `FSUNNonlinSol_FixedPoint`.

The FORTRAN 2003 SUNNONLINSOL_FIXEDPOINT interface module can be accessed with the `use` statement, i.e. `use fsunnonlinsol_fixedpoint_mod`, and linking to the library `libsundials_fsunnonlinsolfixedpoint_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunnonlinsol_fixedpoint_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunnonlinsolfixedpoint_mod` library.

FORTRAN 77 interface functions

For SUNDIALS integrators that include a FORTRAN 77 interface, the SUNNONLINSOL_FIXEDPOINT module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

`FSUNFIXEDPOINTINIT`

Call `FSUNFIXEDPOINTINIT(code, m, ier);`

Description The function `FSUNFIXEDPOINTINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE).

`m` (`int*`) is an integer input specifying the number of acceleration vectors.

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

10.3.4 SUNNonlinearSolver_FixedPoint content

The SUNNONLINSOL_FIXEDPOINT module defines the *content* field of a `SUNNonlinearSolver` as the following structure:

```
struct _SUNNonlinearSolverContent_FixedPoint {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolConvTestFn CTest;

  int       m;
  int      *imap;
  realtype *R;
  realtype *gamma;
  realtype *cvals;
  N_Vector *df;
  N_Vector *dg;
  N_Vector *q;
  N_Vector *Xvecs;
  N_Vector  yprev;
  N_Vector  gy;
  N_Vector  fold;
  N_Vector  gold;
  N_Vector  delta;
```

```
  int       curiter;
  int       maxiters;
  long int  niters;
  long int  nconvfails;
};
```

The following entries of the *content* field are always allocated:

`Sys` - function for evaluating the nonlinear system,

`CTest` - function for checking convergence of the fixed point iteration,

`yprev` - `N_Vector` used to store previous fixed-point iterate,

`gy` - `N_Vector` used to store $G(y)$ in fixed-point algorithm,

`delta` - `N_Vector` used to store difference between successive fixed-point iterates,

`curiter` - the current number of iterations in the solve attempt,

`maxiters` - the maximum number of fixed-point iterations allowed in a solve, and

`niters` - the total number of nonlinear iterations across all solves.

`nconvfails` - the total number of nonlinear convergence failures across all solves.

`m` - number of acceleration vectors,

If Anderson acceleration is requested (i.e., $m > 0$ in the call to `SUNNonlinSol_FixedPoint`), then the following items are also allocated within the *content* field:

`imap` - index array used in acceleration algorithm (length `m`)

`R` - small matrix used in acceleration algorithm (length `m*m`)

`gamma` - small vector used in acceleration algorithm (length `m`)

`cvals` - small vector used in acceleration algorithm (length `m+1`)

`df` - array of `N_Vectors` used in acceleration algorithm (length `m`)

`dg` - array of `N_Vectors` used in acceleration algorithm (length `m`)

`q` - array of `N_Vectors` used in acceleration algorithm (length `m`)

`Xvecs` - `N_Vector` pointer array used in acceleration algorithm (length `m+1`)

`fold` - `N_Vector` used in acceleration algorithm

`gold` - `N_Vector` used in acceleration algorithm

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:

  solverdir 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*`/CMAKE_INSTALL_LIBDIR`, with *instdir* and `CMAKE_INSTALL_LIBDIR` 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 *solverdir* 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 *solverdir*.

- 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 `3.1.3` 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. CMake is continually adding new features, and the latest version can be downloaded 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 *instdir* 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 *solverdir*:

```
% ccmake ../solverdir
```

The default configuration screen is shown in Figure A.1.

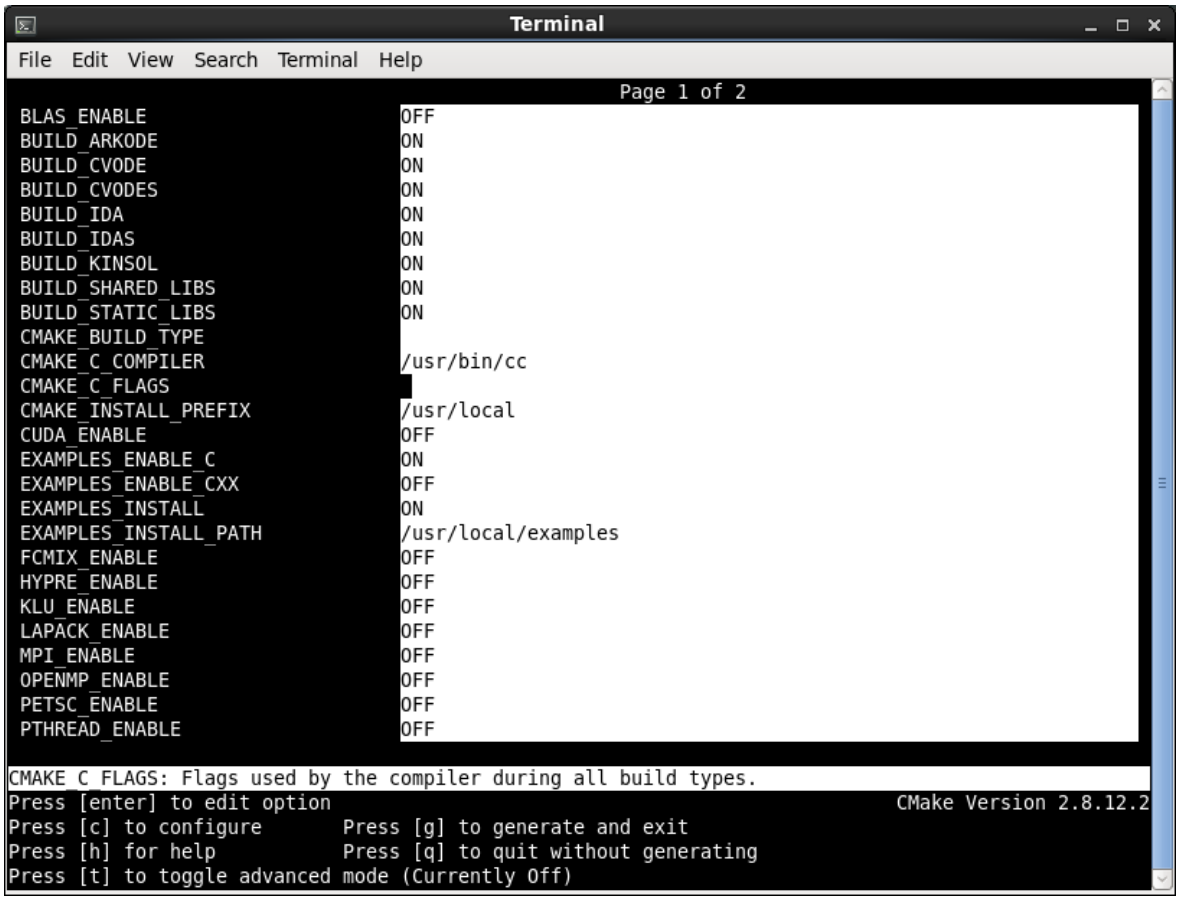

Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

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
```

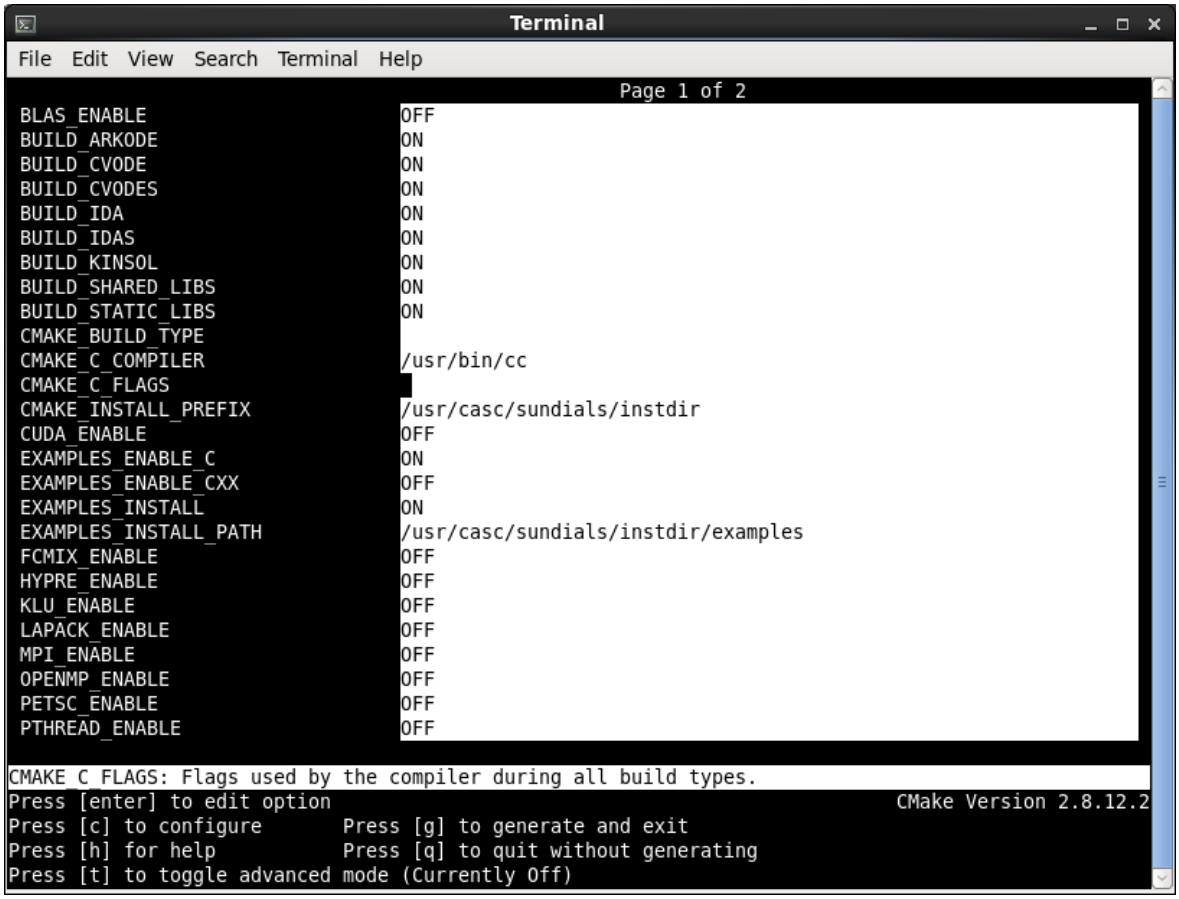

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

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 \
> ../solverdir
% 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 CMAKE_INSTALL_LIBDIR of CMAKE_INSTALL_PREFIX, respectively.

CMAKE_INSTALL_LIBDIR - Library installation directory
Default:
Note: This is the directory within CMAKE_INSTALL_PREFIX that the SUNDIALS libraries will be installed under. The default is automatically set based on the operating system using the GNUInstallDirs CMake module.

Fortran_INSTALL_MODDIR - Fortran module installation directory
Default: fortran

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 F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90/Fortran2003 examples
Default: ON (if F77_INTERFACE_ENABLE or F2003_INTERFACE_ENABLE is ON)

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.

F77_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 77 interfaces
Default: OFF

F2003_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 2003 interfaces
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_C_COMPILER - mpicc program
Default:

`MPI_CXX_COMPILER` - `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_Fortran_COMPILER` - `mpif77` or `mpif90` program
Default:
Note: This option is triggered only if MPI is enabled (`MPI_ENABLE` is ON) and Fortran-C support is enabled (`F77_INTERFACE_ENABLE` or `F2003_INTERFACE_ENABLE` is ON).

`MPIEXEC_EXECUTABLE` - Specify the executable for running MPI programs
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

`OPENMP_DEVICE_ENABLE` - Enable OpenMP device offloading (build the OpenMPDEV nvector) if supported by the provided compiler.
Default: OFF

`SKIP_OPENMP_DEVICE_CHECK` - **advanced option** - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.
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_F77_FUNC_CASE` - **advanced option** - Specify the case to use in the Fortran name-mangling scheme, options are: `lower` or `upper`
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (`lower`) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_UNDERSCORES` must also be set.

`SUNDIALS_F77_FUNC_UNDERSCORES` - **advanced option** - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: `none`, `one`, or `two`
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (`one`) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_CASE` must also be set.

SUNDIALS_INDEX_TYPE - **advanced option** - Integer type used for SUNDIALS indices. The size must match the size provided for the
SUNDIALS_INDEX_SIZE option.
Default:
Note: In past SUNDIALS versions, a user could set this option to INT64_T to use 64-bit integers, or INT32_T to use 32-bit integers. Starting in SUNDIALS 3.2.0, these special values are deprecated. For SUNDIALS 3.2.0 and up, a user will only need to use the SUNDIALS_INDEX_SIZE option in most cases.

SUNDIALS_INDEX_SIZE - Integer size (in bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 64
Note: The build system tries to find an integer type of appropriate size. Candidate 64-bit integer types are (in order of preference): int64_t, __int64, long long, and long. Candidate 32-bit integers are (in order of preference): int32_t, int, and long. The advanced option, SUNDIALS_INDEX_TYPE can be used to provide a type not listed here.

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 interfaces
Default: OFF
SUNDIALS equivalent: F77_INTERFACE_ENABLE/F2003_INTERFACE_ENABLE

XSDK_INDEX_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 32
SUNDIALS equivalent: SUNDIALS_INDEX_SIZE

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/solverdir
%
% 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/solverdir
%
% 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. When building SUNDIALS as a shared library external libraries any used with SUNDIALS must also be build as a shared library or as a static library compiled with the -fPIC flag.

Building with BLAS

SUNDIALS does not utilize BLAS directly but it may be needed by other external libraries that SUNDIALS can be built 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/solverdir
%
% make install
%
```

When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

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/solverdir
%
% make install
%
```

When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options SUNDIALS_F77_FUNC_CASE and SUNDIALS_F77_FUNC_UNDERSCORES *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

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 have been 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 the NVIDIA website: `https://developer.nvidia.com/cuda-downloads`. To enable CUDA, set `CUDA_ENABLE` to `ON`. If CUDA is installed 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

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from `https://github.com/LLNL/RAJA`. SUNDIALS RAJA modules and examples have been tested with RAJA version 0.3. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set `CUDA_ENABLE` and `RAJA_ENABLE` to `ON`. If RAJA is installed in a nonstandard location you will be prompted to set the variable `RAJA_DIR` with the path to the RAJA CMake configuration file. To enable building the RAJA examples set `EXAMPLES_ENABLE_RAJA` to `ON`.

A.1.5 Testing the build and installation

If SUNDIALS was configured with `EXAMPLES_ENABLE_<language>` options to `ON`, then a set of regression tests can be run after building with the `make` command by running:

```
% make test
```

Additionally, if `EXAMPLES_INSTALL` was also set to `ON`, then a set of smoke tests can be run after installing with the `make install` command by running:

```
% make test_install
```

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 *solverdir*
2. Create a separate *builddir*
3. Open a Visual Studio Command Prompt and cd to *builddir*
4. Run cmake-gui ../*solverdir*
   (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*/CMAKE_INSTALL_LIBDIR and *instdir*/include, respectively. The location can be changed by setting the CMake variable CMAKE_INSTALL_PREFIX. Although all installed libraries reside under *libdir*/CMAKE_INSTALL_LIBDIR, the public header files are further organized into subdirectories under *includedir*/include.

The installed libraries and exported header files are listed for reference in Table A.1. 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_matrix.h sundials/sundials_linearsolver.h sundials/sundials_iterative.h sundials/sundials_direct.h sundials/sundials_dense.h sundials/sundials_band.h sundials/sundials_nonlinearsolver.h sundials/sundials_version.h sundials/sundials_mpi_types.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib* libsundials_fnvecserial_mod.*lib* libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module files	fnvector_serial_mod.mod
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib* libsundials_fnvecparallel.a
	Header files	nvector/nvector_parallel.h
NVECTOR_OPENMP	Libraries	libsundials_nvecopenmp.*lib* libsundials_fnvecopenmp_mod.*lib* libsundials_fnvecopenmp.a
	Header files	nvector/nvector_openmp.h
	Module files	fnvector_openmp_mod.mod
NVECTOR_OPENMPDEV	Libraries	libsundials_nvecopenmpdev.*lib*
	Header files	nvector/nvector_openmpdev.h
NVECTOR_PTHREADS	Libraries	libsundials_nvecpthreads.*lib* libsundials_fnvecpthreads_mod.*lib* libsundials_fnvecpthreads.a
	Header files	nvector/nvector_pthreads.h
	Module files	fnvector_pthreads_mod.mod
NVECTOR_PARHYP	Libraries	libsundials_nvecparhyp.*lib*
	Header files	nvector/nvector_parhyp.h

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NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.*lib*
	Header files	nvector/nvector_petsc.h
NVECTOR_CUDA	Libraries Libraries	libsundials_nveccuda.*lib* libsundials_nvecmpicuda.*lib*
	Header files	nvector/nvector_cuda.h nvector/nvector_mpicuda.h nvector/cuda/ThreadPartitioning.hpp nvector/cuda/Vector.hpp nvector/cuda/VectorKernels.cuh
NVECTOR_RAJA	Libraries Libraries	libsundials_nveccudaraja.*lib* libsundials_nveccudampiraja.*lib*
	Header files	nvector/nvector_raja.h nvector/nvector_mpiraja.h nvector/raja/Vector.hpp
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.*lib* libsundials_fsunmatrixband_mod.*lib* libsundials_fsunmatrixband.a
	Header files	sunmatrix/sunmatrix_band.h
	Module files	fsunmatrix_band_mod.mod
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.*lib* libsundials_fsunmatrixdense_mod.*lib* libsundials_fsunmatrixdense.a
	Header files	sunmatrix/sunmatrix_dense.h
	Module files	fsunmatrix_dense_mod.mod
SUNMATRIX_SPARSE	Libraries	libsundials_sunmatrixsparse.*lib* libsundials_fsunmatrixsparse_mod.*lib* libsundials_fsunmatrixsparse.a
	Header files	sunmatrix/sunmatrix_sparse.h
	Module files	fsunmatrix_sparse_mod.mod
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.*lib* libsundials_fsunlinsolband_mod.*lib* libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module files	fsunlinsol_band_mod.mod
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.*lib* libsundials_fsunlinsoldense_mod.*lib* libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h

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	Module files	fsunlinsol_dense_mod.mod
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.*lib* libsundials_fsunlinsolklu_mod.*lib* libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module files	fsunlinsol_klu_mod.mod
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_mod.*lib* libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module files	fsunlinsol_pcg_mod.mod
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.*lib* libsundials_fsunlinsolspbcgs_mod.*lib* libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module files	fsunlinsol_spbcgs_mod.mod
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.*lib* libsundials_fsunlinsolspfgmr_mod.*lib* libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module files	fsunlinsol_spfgmr_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.*lib* libsundials_fsunlinsolspgmr_mod.*lib* libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.*lib* libsundials_fsunlinsolsptfqmr_mod.*lib* libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
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continued from last page			
	Module files	fsunlinsol_sptfqmr_mod.mod	
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.*lib* libsundials_fsunlinsolsuperlumt.a	
	Header files	sunlinsol/sunlinsol_superlumt.h	
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnewton.*lib* libsundials_fsunnonlinsolnewton_mod.*lib* libsundials_fsunnonlinsolnewton.a	
	Header files	sunnonlinsol/sunnonlinsol_newton.h	
	Module files	fsunnonlinsol_newton_mod.mod	
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint.*lib* libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod.*lib*	
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h	
	Module files	fsunnonlinsol_fixedpoint_mod.mod	
CVODE	Libraries	libsundials_cvode.*lib*	libsundials_fcvode.a
	Header files	cvode/cvode.h cvode/cvode_direct.h cvode/cvode_spils.h cvode/cvode_bbdpre.h	cvode/cvode_impl.h cvode/cvode_ls.h cvode/cvode_bandpre.h
	Module files	fcvode_mod.mod	
CVODES	Libraries	libsundials_cvodes.*lib*	
	Header files	cvodes/cvodes.h cvodes/cvodes_direct.h cvodes/cvodes_spils.h cvodes/cvodes_bbdpre.h	cvodes/cvodes_impl.h cvodes/cvodes_ls.h cvodes/cvodes_bandpre.h
ARKODE	Libraries	libsundials_arkode.*lib*	libsundials_farkode.a
	Header files	arkode/arkode.h arkode/arkode_ls.h arkode/arkode_bbdpre.h	arkode/arkode_impl.h arkode/arkode_bandpre.h
IDA	Libraries	libsundials_ida.*lib*	libsundials_fida.a
	Header files	ida/ida.h ida/ida_direct.h ida/ida_spils.h	ida/ida_impl.h ida/ida_ls.h ida/ida_bbdpre.h
IDAS	Libraries	libsundials_idas.*lib*	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_spils.h	idas/idas_impl.h idas/idas_ls.h idas/idas_bbdpre.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a
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	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_spils.h	kinsol/kinsol_impl.h kinsol/kinsol_ls.h kinsol/kinsol_bbdpre.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_NLS_INIT_FAIL	-15	The nonlinear solver's init routine failed.
IDA_NLS_SETUP_FAIL	-16	The nonlinear solver's setup routine failed.
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.

IDALS **linear solver interface**

IDALS_SUCCESS	0	Successful function return.
IDALS_MEM_NULL	-1	The ida_mem argument was NULL.
IDALS_LMEM_NULL	-2	The IDALS linear solver has not been initialized.
IDALS_ILL_INPUT	-3	The IDALS solver is not compatible with the current NVECTOR module, or an input value was illegal.
IDALS_MEM_FAIL	-4	A memory allocation request failed.
IDALS_PMEM_NULL	-5	The preconditioner module has not been initialized.
IDALS_JACFUNC_UNRECVR	-6	The Jacobian function failed in an unrecoverable manner.
IDALS_JACFUNC_RECVR	-7	The Jacobian function had a recoverable error.
IDALS_SUNMAT_FAIL	-8	An error occurred with the current SUNMATRIX module.
IDALS_SUNLS_FAIL	-9	An error occurred with the current SUNLINSOL module.

IDALS_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDALS_LMEMB_NULL	-102	The linear solver was not initialized for the backward phase.

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