User Documentation for IDA v5.0.0-dev.0 (SUNDIALS v5.0.0-dev.0)

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Chapter 1

Introduction

IDA is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [25]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities, CVODES and IDAS.

IDA is a general purpose solver for the initial value problem (IVP) for systems of differential-algebraic equations (DAEs). The name IDA stands for Implicit Differential-Algebraic solver. IDA is based on DASPK [8, 9], but 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; and (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. Thus IDA shares significant modules previously written within CASC at LLNL to support the ordinary differential equation (ODE) solvers CVODE [26, 14] and PVODE [12, 13], and also the nonlinear system solver KINSOL [15].

At present, IDA 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) [37], FGMRES (Flexible Generalized Minimum RESidual) [36], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [38], TFQMR (Transpose-Free Quasi-Minimal Residual) [21], and PCG (Preconditioned Conjugate Gradient) [23] 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.

There are several motivations for choosing the C language for IDA. 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 IDA 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 v5.0.0-dev.0

An additional NVECTOR implementation, NVECTOR_MANYVECTOR, was created to support flexible partitioning of solution data among different processing elements (e.g., CPU + GPU) or for multi-physics problems that couple distinct MPI-based simulations together (see Section 6.12 for more details). This implementation is accompanied by additions to user documentation and SUNDIALS examples.

Eleven new optional vector operations have been added to the NVECTOR API to support the new NVECTOR_MANYVECTOR implementation (see Chapter 6 for more details). Two of the operations, N_VGetCommunicator and N_VGetLength, must be implemented by subvectors that are combined to create an NVECTOR_MANYVECTOR, but are not used outside of this context. The remaining nine operations are optional local reduction operations intended to eliminate unnecessary latency when performing vector reduction operations (norms, etc.) on distributed memory systems. The optional local reduction vector operations are N_VDotProdLocal, N_VMaxNormLocal, N_VMinLocal, N_VL1NormLocal, N_VWSqrSumLocal, N_VWSqrSumMaskLocal, N_VInvTestLocal, N_VConstrMaskLocal, and N_VMinQuotientLocal. If an NVECTOR implementation defines any of the local operations as NULL, then the NVECTOR_MANYVECTOR will call standard NVECTOR operations to complete the computation.

A new SUNMATRIX and SUNLINSOL implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS.

A new operation, SUNMatMatvecSetup, was added to the SUNMATRIX API. Users who have implemented custom SUNMATRIX modules will need to at least update their code to set the corresponding ops structure member, matvecsetup, to NULL.

The generic SUNMATRIX API now defines error codes to be returned by SUNMATRIX operations. Operations which return an integer flag indiciating success/failure may return different values than previously.

Changes in v4.1.0

An additional NVECTOR implementation was added for the Tpetra vector from the Trilinos library to facilitate interoperability between SUNDIALS and Trilinos. This implementation is accompanied by additions to user documentation and SUNDIALS examples.

A bug was fixed where a nonlinear solver object could be freed twice in some use cases.

The EXAMPLES_ENABLE_RAJA CMake option has been removed. The option EXAMPLES_ENABLE_CUDA enables all examples that use CUDA including the RAJA examples with a CUDA back end (if the RAJA NVECTOR is enabled).

The implementation header file ida_impl.h is no longer installed. This means users who are directly manipulating the IDAMem structure will need to update their code to use IDA's public API.

Python is no longer required to run make test and make test_install.

Changes in v4.0.2

Added information on how to contribute to SUNDIALS and a contributing agreement.

Moved definitions of DLS and SPILS backwards compatibility functions to a source file. The symbols are now included in the IDA library, libsundials_ida.

Changes in v4.0.1

No changes were made in this release.

Changes in v4.0.0

IDA's 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 8. All IDA 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 and FORTRAN routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon. Additionally, we note that FORTRAN users, however, may need to enlarge their `iout` array of optional integer outputs, and update the indices that they query for certain linear-solver-related statistics.

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 IDA 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 9 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 IDA example programs have been updated to use generic SUNNONLINSOL modules.

By default IDA uses the SUNNONLINSOL_NEWTON module. Since IDA 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 IDA. For details on attaching a user-supplied nonlinear solver to IDA see Chapter 4. Additionally, the example program `idaRoberts_dns.c` explicitly creates an attaches a SUNNONLIN-SOL_NEWTON object to demonstrate the process of creating and attaching a nonlinear solver module (note this is not necessary in general as IDA uses the SUNNONLINSOL_NEWTON module by default).

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 6 for more details). The new operations are intended to increase data reuse in vector operations, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. The fused 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 §6.10 for more details.

Changes in v3.2.1

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 v3.2.0

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 deprecated. 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 v3.1.2

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 SUNLinearSolver 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 v3.1.1

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 SUNLINSOL 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.

- Fixed compilation issue with GCC 7.3.0 and Fortran programs that do not require a SUNMATRIX module (e.g., iterative linear solvers).

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

Changes in v3.1.0

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 v3.0.0

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 v2.9.0

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. Also, corrections were made to three Fortran interface functions.

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

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.

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

Changes in v2.8.0

Two major additions were made to the linear system solvers that are available for use with the IDA 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 IDA.

Otherwise, only relatively minor modifications were made to IDA:

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`.

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

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 FIDA optional input routines `FIDASETIIN`, `FIDASETRIN`, and `FIDASETVIN`, the optional fourth argument `key_length` was removed, with hardcoded key string lengths passed to all `strncmp` tests.

In all FIDA examples, integer declarations were revised so that those which must match a C type `long int` are declared `INTEGER*8`, and a comment was added about the type match. All other integer declarations are just `INTEGER`. Corresponding minor corrections were made to the user guide.

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 v2.7.0

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.

A large number of minor errors have been fixed. Among these are the following: After the solver memory is created, it is set to zero before being filled. To be consistent with IDAS, IDA uses the function `IDAGetDky` for optional output retrieval. 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 SUNDI-ALS_USE_GENERIC_MATH, so that the parameter GENERIC_MATH_LIB is either defined (with no value) or not defined.

Changes in v2.6.0

Two new features were added in this release: (a) a new linear solver module, based on BLAS and LAPACK for both dense and banded matrices, and (b) option to specify which direction of zero-crossing is to be monitored while performing rootfinding.

The user interface has been further refined. Some of the API changes involve: (a) a reorganization of all linear solver modules into two families (besides the already present family of scaled preconditioned iterative linear solvers, the direct solvers, including the new LAPACK-based ones, were also organized into a *direct* family); (b) maintaining a single pointer to user data, optionally specified through a `Set`-type function; (c) a general streamlining of the band-block-diagonal preconditioner module distributed with the solver.

Changes in v2.5.0

The main changes in this release involve a rearrangement of the entire SUNDIALS source tree (see §3.1). At the user interface level, the main impact is in the mechanism of including SUNDIALS header files which must now include the relative path (e.g. `#include <cvode/cvode.h>`). Additional changes were made to the build system: all exported header files are now installed in separate subdirectories of the installation *include* directory.

A bug was fixed in the internal difference-quotient dense and banded Jacobian approximations, related to the estimation of the perturbation (which could have led to a failure of the linear solver when zero components with sufficiently small absolute tolerances were present).

The user interface to the consistent initial conditions calculations was modified. The `IDACalcIC` arguments `t0`, `yy0`, and `yp0` were removed and a new function, `IDAGetconsistentIC` is provided (see §4.5.5 and §4.5.10.3 for details).

The functions in the generic dense linear solver (`sundials_dense` and `sundials_smalldense`) were modified to work for rectangular $m \times n$ matrices ($m \leq n$), while the factorization and solution functions were renamed to `DenseGETRF/denGETRF` and `DenseGETRS/denGETRS`, respectively. The factorization and solution functions in the generic band linear solver were renamed `BandGBTRF` and `BandGBTRS`, respectively.

Changes in v2.4.0

FIDA, a FORTRAN-C interface module, was added (for details see Chapter 5).

IDASPBCG and IDASPTFQMR modules have been added to interface with the Scaled Preconditioned Bi-CGstab (SPBCGS) and Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR) linear solver modules, respectively (for details see Chapter 4). At the same time, function type names for Scaled Preconditioned Iterative Linear Solvers were added for the user-supplied Jacobian-times-vector and preconditioner setup and solve functions.

The rootfinding feature was added, whereby the roots of a set of given functions may be computed during the integration of the DAE system.

A user-callable routine was added to access the estimated local error vector.

The deallocation functions now take as arguments the address of the respective memory block pointer.

To reduce the possibility of conflicts, the names of all header files have been changed by adding unique prefixes (`ida_` and `sundials_`). When using the default installation procedure, the header files are exported under various subdirectories of the target `include` directory. For more details see Appendix A.

Changes in v2.3.0

The user interface has been further refined. Several functions used for setting optional inputs were combined into a single one. An optional user-supplied routine for setting the error weight vector was added. Additionally, to resolve potential variable scope issues, all SUNDIALS solvers release user data right after its use. The build systems has been further improved to make it more robust.

Changes in v2.2.2

Minor corrections and improvements were made to the build system. A new chapter in the User Guide was added — with constants that appear in the user interface.

Changes in v2.2.1

The changes in this minor SUNDIALS release affect only the build system.

Changes in v2.2.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the `iopt` and `ropt` arrays. Instead, IDA now provides a set of routines (with prefix `IDASet`) to change the default values for various quantities controlling the solver and a set of extraction routines (with prefix `IDAGet`) to extract statistics after return from the main solver routine. Similarly, each linear solver module provides its own set of `Set`- and `Get`-type routines. For more details see §4.5.8 and §4.5.10.

Additionally, the interfaces to several user-supplied routines (such as those providing Jacobians and preconditioner information) were simplified by reducing the number of arguments. The same information that was previously accessible through such arguments can now be obtained through `Get`-type functions.

Installation of IDA (and all of SUNDIALS) has been completely redesigned and is now based on configure scripts.

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 IDA for the solution of initial value problems for systems of DAEs, along with short descriptions of preconditioning (§2.2) and rootfinding (§2.3).

- The following chapter describes the structure of the SUNDIALS suite of solvers (§3.1) and the software organization of the IDA solver (§3.2).

- Chapter 4 is the main usage document for IDA for C applications. It includes a complete description of the user interface for the integration of DAE initial value problems.

- In Chapter 5, we describe FIDA, an interface module for the use of IDA with FORTRAN applications.

- Chapter 6 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, as well as details on the NVECTOR implementations provided with SUNDIALS.

- Chapter 7 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 (§7.5), a banded implementation (§7.6) and a sparse implementation (§7.7).

- Chapter 8 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 9 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 IDA, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from IDA 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 IDADLS, are written in all capitals. Usage and installation instructions that constitute important warnings are marked with a triangular symbol in the margin.

Acknowledgments. We wish to acknowledge the contributions to previous versions of the IDA code and user guide of Allan G. Taylor.

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1.3.3 SUNDIALS Release Numbers

```
LLNL-CODE-667205   (ARKODE)
UCRL-CODE-155951   (CVODE)
UCRL-CODE-155950   (CVODES)
UCRL-CODE-155952   (IDA)
UCRL-CODE-237203   (IDAS)
LLNL-CODE-665877   (KINSOL)
```

Chapter 2

Mathematical Considerations

IDA 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.)

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, IDA provides a routine that computes consistent initial conditions from a user's initial guess [9]. 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 IDA 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 IDA is the variable-order, variable-coefficient BDF (Backward Differentiation Formula), in fixed-leading-coefficient form [5]. The method order ranges from 1 to 5, with the BDF of order q given by the multistep formula

$$\sum_{i=0}^{q} \alpha_{n,i} y_{n-i} = h_n \dot{y}_n \,, \tag{2.2}$$

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 (2.2) to the DAE system (2.1) results in a nonlinear algebraic system to be solved at each step:

$$G(y_n) \equiv F\left(t_n, \, y_n, \, h_n^{-1} \sum_{i=0}^{q} \alpha_{n,i} y_{n-i}\right) = 0 \,. \tag{2.3}$$

By default IDA solves (2.3) with a Newton iteration but IDA also allows for user-defined nonlinear solvers (see Chapter 9). Each Newton iteration requires the solution of a linear system of the form

$$J[y_{n(m+1)} - y_{n(m)}] = -G(y_{n(m)}) , \tag{2.4}$$

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

$$J = \frac{\partial G}{\partial y} = \frac{\partial F}{\partial y} + \alpha \frac{\partial F}{\partial \dot{y}} , \tag{2.5}$$

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, IDA provides several choices, including the option of a user-supplied linear solver module (see Chapter 8). 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 [16, 1], or the thread-enabled SuperLU_MT sparse solver library [31, 18, 3] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of IDA],

- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver with or without restarts,

- SPFGMR, a scaled preconditioned FGMRES (Flexible Generalized Minimal Residual method) solver with or without restarts,

- 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 [7]. For the *spils* linear solvers with IDA, 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, IDA 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

$$W_i = 1/[\text{RTOL} \cdot |y_i| + \text{ATOL}_i] . \tag{2.6}$$

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 IDA 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

$$S\|\delta_m\| < 0.33, \tag{2.7}$$

where $S = R/(R-1)$ whenever $m > 1$ and $R \le 0.9$. The user has the option of changing the constant in the convergence test from its default value of 0.33. The quantity S is set to $S = 20$ initially and whenever J or P is updated, and it is reset to $S = 100$ on a step with $\alpha \neq \bar{\alpha}$. Note that at $m = 1$, the convergence test (2.7) 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 (2.5) can be either supplied by the user or have IDA compute one internally by difference quotients. In the latter case, we use the approximation

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

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 (2.6). 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, IDA 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, IDA 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 IDA is

$$\max\{|C|, \bar{C}\}\|\Delta_n\| \leq 1\,. \tag{2.8}$$

A user option is available by which the algebraic components of the error vector are omitted from the test (2.8), if these have been so identified.

In IDA, 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 (2.8) 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, IDA 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 IDA (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 IDA 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 (2.8) 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, IDA uses $\eta = 0.25$, and on the third and subsequent failures it uses $q = 1$ and $\eta = 0.25$. After 10 failures, IDA 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, IDA 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:

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

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 [5] for details.

IDA 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, IDA 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, IDA takes steps until a user-defined output value $t = t_{\text{out}}$ is overtaken, and then computes $y(t_{\text{out}})$ 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 IDA not to integrate past a given stopping point $t = t_{\text{stop}}$.

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), IDA 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 IDA, 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 [7] for an extensive study of preconditioners for reaction-transport systems).

Typical preconditioners used with IDA 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 IDA solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (2.1), IDA 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 IDA. 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 [24]. In addition, each time g is computed, IDA 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, IDA 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, IDA stops and reports an error. This way, each time IDA 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, IDA 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 $\tau/2$.

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 IDA organization

The IDA 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 IDA package is shown in Figure 3.3. The central integration module, implemented in the files `ida.h`, `ida_impl.h`, and `ida.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.

IDA utilizes generic linear and nonlinear solver modules defined by the SUNLINSOL API (see Chapter 8) and SUNNONLINSOL API (see Chapter 9) respectively. As such, IDA 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, a linear system solver interface is specified, and invoked as needed during the integration. While SUNDIALS includes a fixed-point nonlinear solver module, it is not currently supported in IDA (note the fixed-point module is listed in Figure 3.1 but not Figure 3.3).

IDA now has a single unified linear solver interface, IDALS, supporting both direct and iterative linear solvers built using the generic SUNLINSOL API (see Chapter 8). These solvers may utilize a
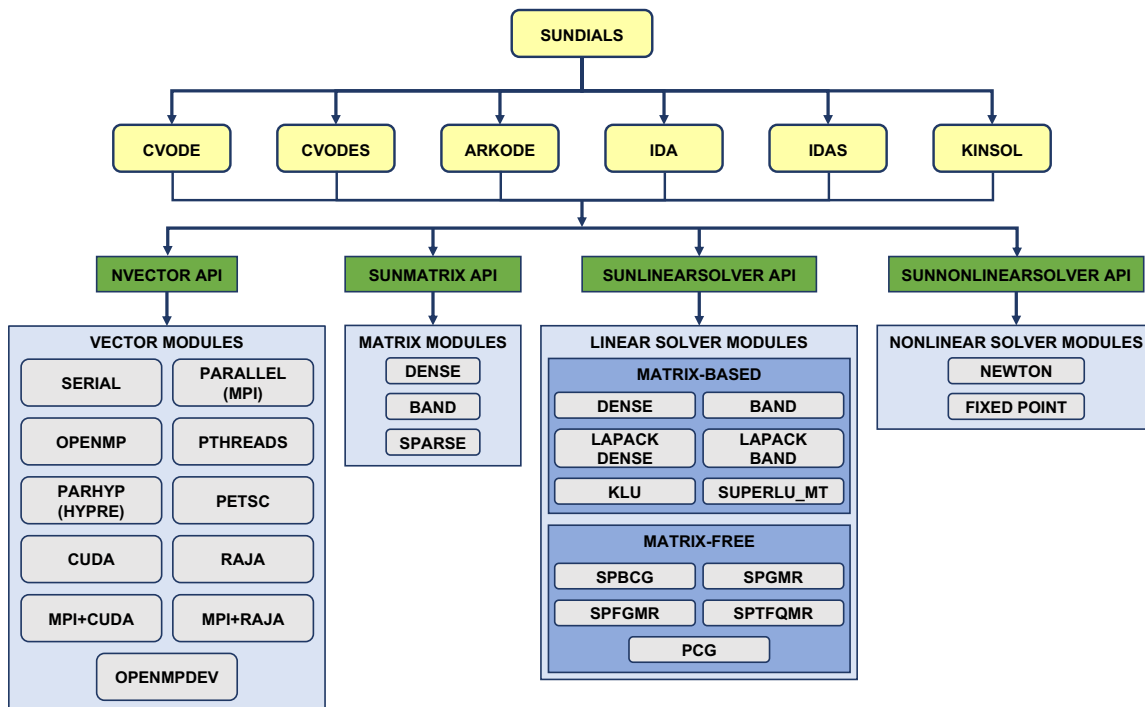
Figure 3.1: High-level diagram of the SUNDIALS suite

SUNMATRIX object (see Chapter 7) for storing Jacobian information, or they may be matrix-free. Since IDA can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to IDA 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 [7, 11], together with the example and demonstration programs included with IDA, offer considerable assistance in building preconditioners.

IDA's 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 IDA module to each of the four associated functions is fixed, thus allowing the central module to be completely independent of the linear system method.

IDA 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 IDA 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 IDA package, and so, in this
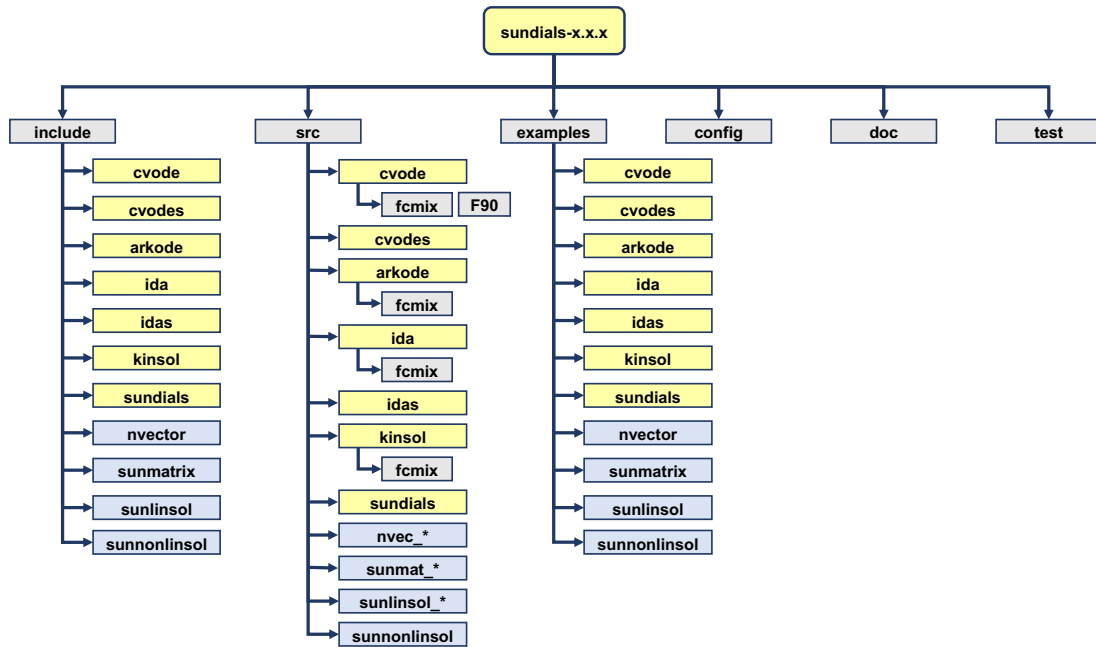
(a) Directory structure of the SUNDIALS source tree
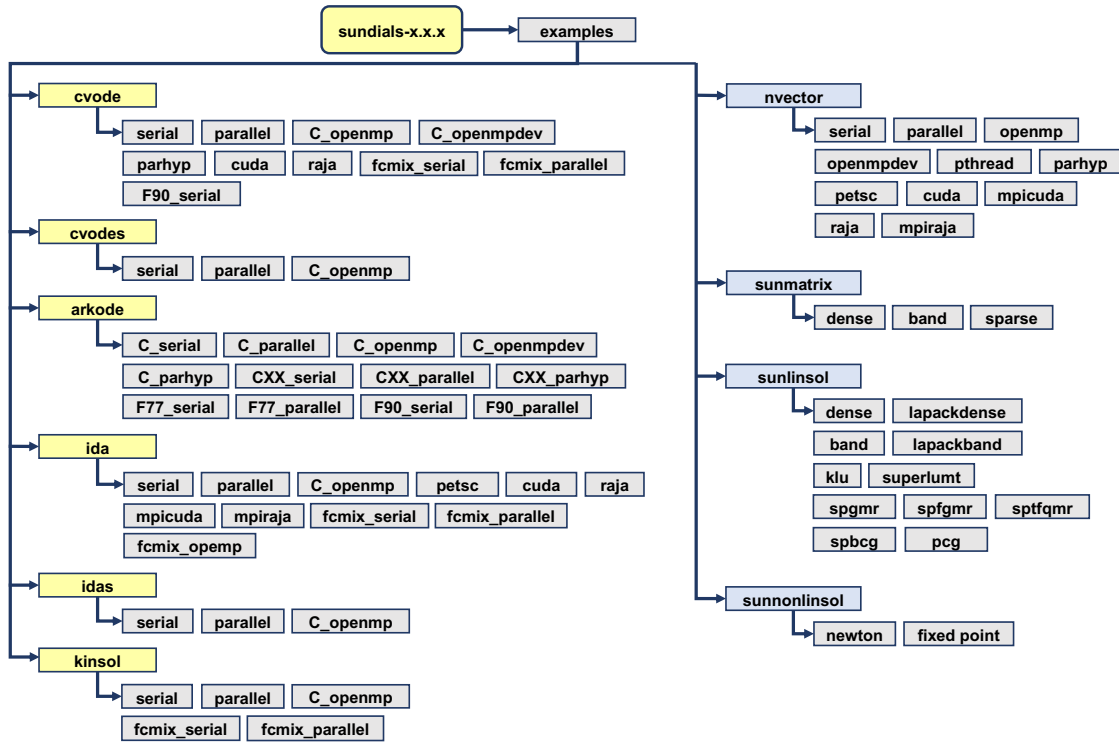
(b) Directory structure of the SUNDIALS examples

Figure 3.2: Organization of the SUNDIALS suite
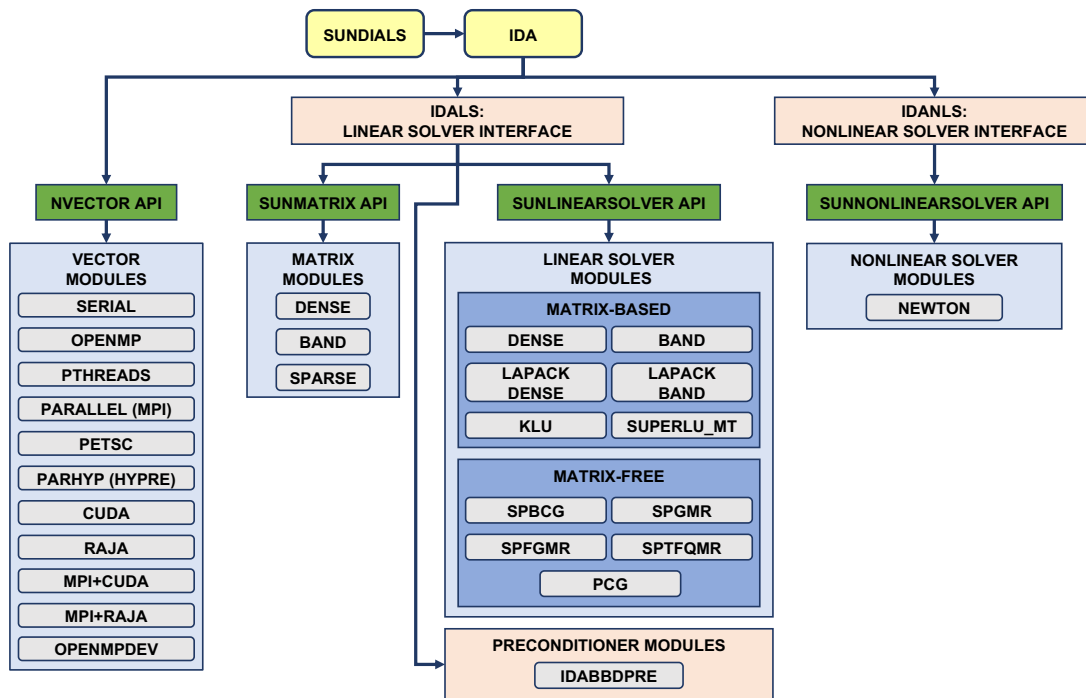
Figure 3.3: Overall structure diagram of the IDA package. Modules specific to IDA begin with "IDA" (IDALS, IDABBDPRE, and IDANLS), all other items correspond to generic solver and auxiliary modules. Note also that the LAPACK, KLU and SUPERLUMT support is through interfaces to external packages. Users will need to download and compile those packages independently.

respect, it is reentrant. State information specific to the linear solver is saved in a separate structure, a pointer to which resides in the IDA memory structure. The reentrancy of IDA 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 IDA for C Applications

This chapter is concerned with the use of IDA 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 IDA user-callable functions, and description of user-supplied functions.

The sample programs described in the companion document [27] 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 IDA package.

Users with applications written in FORTRAN should see Chapter 5, which describes the FORTRAN/C interface module.

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 7) and each SUNLINSOL module (Chapter 8). 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 7 and 8 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.

IDA 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 IDA, 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 IDA. The relevant library files are

- *libdir*/`libsundials_ida.`*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/ida`

- *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:

- `ida/ida.h`, the header file for IDA, 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 `ida.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 6 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 9 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 (2.4) (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 IDA are:

- Direct linear solvers:

  - `sunlinsol/sunlinsol_dense.h`, which is used with the dense linear solver module, SUN-LINSOL_DENSE;

  - `sunlinsol/sunlinsol_band.h`, which is used with the banded linear solver module, SUN-LINSOL_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 idaFoodWeb_kry_p example (see [27]), 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 6, 7, 8, and 9 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 §6.2-6.5 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 §6.6 and §6.7 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 §6.8-6.9 for details.

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

4. **Create IDA object**

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

5. **Initialize IDA solver**

   Call `IDAInit(...)` to provide required problem specifications (residual function, initial time, and initial conditions), allocate internal memory for IDA, and initialize IDA. `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 calling 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 8.

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 8 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 IDA. 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 imple-
    mentation (e.g., NLS = SUNNonlinSol_***(...); where *** is the name of the nonlinear solver
    (see Chapter 9 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 IDA, otherwise the optional inputs
    will be overridden by IDA defaults. See Chapter 9 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 IDA.

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 8 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 IDA 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 IDA. 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 IDA 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 IDA memory block created and allocated by the first two calls.

| `IDACreate` |

Call	`ida_mem = IDACreate();`
Description	The function `IDACreate` instantiates an IDA solver object.
Arguments	`IDACreate` has no arguments.
Return value	If successful, `IDACreate` returns a pointer to the newly created IDA 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 IDA.
Arguments	`ida_mem` (`void *`) pointer to the IDA 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 IDA 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 IDA memory block (of type `void *`).
Return value	The function `IDAFree` has no return value.

4.5.2 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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. (2.6).

Arguments   ida_mem (void *) pointer to the IDA 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 IDA 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 `idaRoberts_dns` in the IDA package, and the discussion of it in the IDA Examples document [27]. 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 IDA, 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) IDA 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, a if the nonlinear solver requires the solution of linear systems of the from (2.4) (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 IDA 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 IDA, 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 7 and 8.

Once this solver object has been constructed, the user should attach it to IDA via a call to `IDASetLinearSolver`. The first argument passed to this function is the IDA 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 IDA 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 IDA, initializing the IDALS linear solver interface.
Arguments	`ida_mem` (`void *`) pointer to the IDA memory block.
	`LS` (`SUNLinearSolver`) SUNLINSOL object to use for solving linear systems of the form (2.4.
	`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 7 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 IDA uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNON-LINSOL_NEWTON module (see §9.2). To specify a different nonlinear solver in IDA, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to IDA by calling `IDASetNonlinearSolver`, as documented below.

When changing the nonlinear solver in IDA, `IDASetNonlinearSolver` must be called after `IDAInit`. If any calls to `IDASolve` have been made, then IDA 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 IDA memory pointer returned by `IDACreate` and the second argument is the SUNNONLINSOL object to use for solving the nonlinear system 2.3. A call to this function attaches the nonlinear solver to the main IDA 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 IDA.
Arguments	`ida_mem` (`void *`) pointer to the IDA 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.

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. [9].) 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 IDA 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, IDA 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 IDA 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   IDA 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 IDA 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 IDA 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 $y(\texttt{tout})$ and $\dot{y}(\texttt{tout})$. 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 $t = \texttt{tret}$, 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 $= y(\texttt{tout})$, ypret $= \dot{y}(\texttt{tout})$.

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. See §4.5.8.1 for more information.
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.

If a stop time is enabled (through a call to `IDASetStopTime`), then `IDASolve` returns the solution at `tstop`. Once the integrator returns at a stop time, any future testing for `tstop` is disabled (and can be reenabled only though a new call to `IDASetStopTime`).

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 IDA solver. IDA 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 IDA which are then described in detail in the remainder of this section. For the most casual use of IDA, 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.

IDASetErrFile

Call   flag = IDASetErrFile(ida_mem, errfp);

Table 4.2: Optional inputs for IDA and IDALS

Optional input	Function name	Default
IDA 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
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
IDA 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`	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

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

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

Arguments `ida_mem`   (`void *`) pointer to the IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA memory block.
	`hin` (`realtype`) value of the initial step size to be attempted. Pass 0.0 to have IDA 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, IDA 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 IDA 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 IDA 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.

Once the integrator returns at a stop time, any future testing for `tstop` is disabled (and can be reenabled only though a new call to **IDASetStopTime**).

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 IDA 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 10.

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 IDA 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 4.

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 IDA 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. (2.7).

Arguments   `ida_mem` (`void *`) pointer to the IDA 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 IDA 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. [5] 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 IDA 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 IDA memory block.
	`constraints` (`N_Vector`) vector of constraint flags. If `constraints[i]` is
	$\quad$ 0.0 then no constraint is imposed on y_i.
	$\quad$ 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 $y_i \leq 0.0$.
	$\quad$ 2.0 then y_i will be constrained to be $y_i > 0.0$.
	-2.0 then y_i will be constrained to be $y_i < 0.0$.
Return value	The return value `flag` (of type `int`) is one of
	IDA_SUCCESS The optional value has been successfully set.
	IDA_MEM_NULL The `ida_mem` pointer is `NULL`.
	IDA_ILL_INPUT The constraints vector contains illegal values.
Notes	The presence of a non-`NULL` constraints vector that is not 0.0 in all components will cause constraint checking to be performed. However, a call with 0.0 in all components of `constraints` will result in an illegal input return.

4.5.8.2   Linear solver interface optional input functions

The mathematical explanation of the linear solver methods available to IDA 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 IDA 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 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 itera-
              tions allowed in any one attempt to solve the initial conditions calculation problem.

Arguments   ida_mem (void *) pointer to the IDA 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 back-
              tracks allowed in any Newton iteration, when solving the initial conditions calculation
              problem.

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

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

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

              IDA_SUCCESS   The optional value has been successfully set.

              IDA_MEM_NULL   The ida_mem pointer is NULL.

              IDA_ILL_INPUT maxbacks is non-positive.

Notes   The default value is 100.

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 IDA 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 IDA 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 IDA 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 IDA 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   IDA 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), IDA 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 IDA.

   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 kth derivative of y for
              any value of t in the last internal step taken by IDA. 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 IDA 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

IDA provides an extensive list of functions that can be used to obtain solver performance information.
Table 4.3 lists all optional output functions in IDA, 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 IDA 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.

SUNDIALSGetVersion

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

Description   The function `SUNDIALSGetVersion` fills a character array with SUNDIALS version infor-
              mation.

Arguments   `version` (`char *`) character array to hold the SUNDIALS version information.

              `len`   (`int`) allocated length of the `version` character array.

Table 4.3: Optional outputs from IDA and IDALS

Optional output	Function name
IDA main solver	
Size of IDA 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`
IDA 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`

Return value   If successful, SUNDIALSGetVersion returns 0 and version contains the SUNDIALS ver-
                sion 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

IDA 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 IDA 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, ad-
ditional 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 IDA real and integer workspace sizes.

Arguments   ida_mem (void *) pointer to the IDA memory block.
                lenrw   (long int) number of real values in the IDA workspace.
                leniw   (long int) number of integer values in the IDA 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 $m = \max(\texttt{maxord}, 3)$, and N_r is the number of real words in one `N_Vector` ($\approx N$).

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

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

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

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

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 IDA memory block.
	`nsteps` (`long int`) number of steps taken by IDA.
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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 (if from IDASolve), or the last value of the artificial step size h (if from IDACalcIC).

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

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

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

IDAGetCurrentStep

Call	flag = IDAGetCurrentStep(ida_mem, &hcur);
Description	The function IDAGetCurrentStep returns the integration step size to be attempted on the next internal step.
Arguments	ida_mem (void *) pointer to the IDA 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 IDA 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 IDA to ensure that the step size is within the prescribed bounds ($h_{\min} \leq h_0 \leq h_{\max}$), 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 IDA 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 IDA 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. (2.6) (or by the user's **IDAEwtFn**).
Arguments	`ida_mem` (`void *`) pointer to the IDA 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 IDA 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 IDA integrator statistics as a group.
Arguments	`ida_mem` (`void *`) pointer to the IDA memory block.
	`nsteps` (`long int`) cumulative number of steps taken by IDA.
	`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 IDA 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 IDA 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 IDA nonlinear solver statistics as a group.

Arguments   `ida_mem` (`void *`) pointer to the IDA 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 IDA constant corresponding to `flag`.

Arguments   The only argument, of type `int`, is a return flag from an IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA memory block.

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

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 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 IDA memory block.
               njvevals (long int) the cumulative number of calls to jtimes.

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 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 IDA 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 IDALS 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 $1 \leq$ `lsflag` $\leq N$ (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 IDA reinitialization function

The function `IDAReInit` reinitializes the main IDA 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 IDA.

Arguments   `ida_mem` (`void *`) pointer to the IDA 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 IDA memory block was not initialized through a previous call to
                IDACreate.

IDA_NO_MALLOC Memory space for the IDA 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 func-
             tion.

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, IDA 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 solu-
             tion 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.)

             Allocation of memory for yp is handled within IDA.

### 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 IDA and its sub-modules.

Arguments   `error_code` is the error code.

          `module`       is the name of the IDA 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 $\| v \|_{\mathrm{WRMS}} = \sqrt{(1/N) \sum_1^N (W_i \cdot v_i)^2}$. These weights will used in place of those defined by Eq. (2.6). 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 IDA.

         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,`<br>`                         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 IDA.

## 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,`<br>`                          N_Vector yy, N_Vector yp, N_Vector rr,`<br>`                          SUNMatrix Jac, void *user_data,`<br>`                          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. (2.5).

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 ($\alpha$ in Eq. (2.5) ).

             `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 $\alpha$ in (2.5).

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 7 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 §7.5.

**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 §7.6.

**sparse**:

A user-supplied sparse Jacobian function must load the `Neq` × `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 docu-
mented in §7.7.

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 approxi-
              mation to it) and a given vector v, where $J$ is defined by Eq. (2.5).

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 ($\alpha$ in Eq. (2.5) ).

              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:

---

| `IDALsJacTimesSetupFn` |
| --- |

| | |
| --- | --- |
| Definition | `typedef int (*IDALsJacTimesSetupFn)(realtype tt, N_Vector yy,`<br>`N_Vector yp, N_Vector rr,`<br>`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 ($\alpha$ in Eq. (2.5) ). |
| | `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,`<br>`N_Vector yp, N_Vector rr,`<br>`N_Vector rvec, N_Vector zvec,`<br>`realtype cj, realtype delta,`<br>`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 ($\alpha$ in Eq. (2.5) ). |
| | 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,`<br>`                                 N_Vector yp, N_Vector rr,`<br>`                                 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 ($\alpha$ in Eq. (2.5) ). |
| | 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  A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel DAE solver such as IDA 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 (2.4) 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 [29] and is included in a software module within the IDA 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 $\mathtt{mudq} + \mathtt{mldq} +2$ evaluations of $G_m$, but only a matrix of bandwidth $\mathtt{mukeep} + \mathtt{mlkeep} +1$ 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 $\mathtt{mukeep}$ and $\mathtt{mlkeep}$ while keeping $\mathtt{mudq}$ and $\mathtt{mldq}$ 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 $\mathtt{Gres}$ (of type $\mathtt{IDABBDLocalFn}$) 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 $\mathtt{Gcomm}$ (of type $\mathtt{IDABBDCommFn}$) which performs all inter-process communication necessary to evaluate the approximate residual $G$. These are in addition to the user-supplied residual function $\mathtt{res}$. Both functions take as input the same pointer $\mathtt{user\_data}$ as passed by the user to $\mathtt{IDASetUserData}$ and passed to the user's function $\mathtt{res}$. The user is responsible for providing space (presumably within $\mathtt{user\_data}$) for components of $\mathtt{yy}$ and $\mathtt{yp}$ that are communicated by $\mathtt{Gcomm}$ from the other processors, and that are then used by $\mathtt{Gres}$, which should not do any communication.

---

| $\boxed{\mathtt{IDABBDLocalFn}}$ |

Definition
```
typedef int (*IDABBDLocalFn)(sunindextype Nlocal, realtype tt,
                              N_Vector yy, N_Vector yp, N_Vector gval,
                              void *user_data);
```

Purpose         This $\mathtt{Gres}$ function computes $G(t, y, \dot{y})$. It loads the vector $\mathtt{gval}$ as a function of $\mathtt{tt}$, $\mathtt{yy}$, and $\mathtt{yp}$.

Arguments       $\mathtt{Nlocal}$      is the local vector length.

                $\mathtt{tt}$          is the value of the independent variable.

                $\mathtt{yy}$          is the dependent variable.

                $\mathtt{yp}$          is the derivative of the dependent variable.

                $\mathtt{gval}$        is the output vector.

                $\mathtt{user\_data}$ is a pointer to user data, the same as the $\mathtt{user\_data}$ parameter passed to $\mathtt{IDASetUserData}$.

Return value    An $\mathtt{IDABBDLocalFn}$ 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 $\mathtt{gval}$ has already been done, and this data is accessible within $\mathtt{user\_data}$.

                The case where $G$ is mathematically identical to $F$ is allowed.

---

IDABBDCommFn

| | |
|---|---|
| Definition | `typedef int (*IDABBDCommFn)(sunindextype Nlocal, realtype tt,`<br>`                                    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`.<br><br>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 `ida_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 IDA object**

5. **Initialize IDA 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 IDA 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 ID-ABBDPRE preconditioner.
Arguments	`ida_mem` (`void *`) pointer to the IDA 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 IDA 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 IDA 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 IDA 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 IDA 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 IDA output (see §4.5.10.2), and `npsolves` and `nrevalsLS` are linear solver optional outputs (see §4.5.10.5).

Chapter 5

FIDA, an Interface Module for FORTRAN Applications

The FIDA interface module is a package of C functions which support the use of the IDA solver, for the solution of DAE systems, in a mixed FORTRAN/C setting. While IDA is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in FORTRAN. This package provides the necessary interface to IDA for all supplied serial and parallel NVECTOR implementations.

5.1   Important note on portability

In this package, the names of the interface functions, and the names of the FORTRAN user routines called by them, appear as dummy names which are mapped to actual values by a series of definitions in the header files. By default, those mapping definitions depend in turn on the C macro `F77_FUNC` defined in the header file `sundials_config.h`. The mapping defined by `F77_FUNC` in turn transforms the C interface names to match the name-mangling approach used by the supplied Fortran compiler.

By "name-mangling", we mean that due to the case-independent nature of the FORTRAN language, FORTRAN compilers convert all subroutine and object names to use either all lower-case or all upper-case characters, and append either zero, one or two underscores as a prefix or suffix to the name. For example, the FORTRAN subroutine `MyFunction()` will be changed to one of `myfunction`, `MYFUNCTION`, `myfunction__`, `MYFUNCTION_`, and so on, depending on the FORTRAN compiler used.

SUNDIALS determines this name-mangling scheme at configuration time (see Appendix A).

5.2   Fortran Data Types

Throughout this documentation, we will refer to data types according to their usage in C. The equivalent types to these may vary, depending on your computer architecture and on how SUNDIALS was compiled (see Appendix A). A FORTRAN user should first determine the equivalent types for their architecture and compiler, and then take care that all arguments passed through this FORTRAN/C interface are declared of the appropriate type.

Integers: While SUNDIALS uses the configurable `sunindextype` type as the integer type for vector and matrix indices for its C code, the FORTRAN interfaces are more restricted. The `sunindextype` is only used for index values and pointers when filling sparse matrices. As for C, the `sunindextype` can be configured to be a 32- or 64-bit signed integer by setting the variable `SUNDIALS_INDEX_TYPE` at compile time (See Appendix A). The default value is `int64_t`. A FORTRAN user should set this variable based on the integer type used for vector and matrix indices in their FORTRAN code. The corresponding FORTRAN types are:

- `int32_t` – equivalent to an `INTEGER` or `INTEGER*4` in FORTRAN

- int64_t – equivalent to an INTEGER*8 in FORTRAN

In general, for the FORTRAN interfaces in SUNDIALS, flags of type int, vector and matrix lengths, counters, and arguments to *SETIN() functions all have long int type, and sunindextype is only used for index values and pointers when filling sparse matrices. Note that if an F90 (or higher) user wants to find out the value of sunindextype, they can include sundials_fconfig.h.

   Real numbers: As discussed in Appendix A, at compilation SUNDIALS allows the configuration option SUNDIALS_PRECISION, that accepts values of single, double or extended (the default is double). This choice dictates the size of a realtype variable. The corresponding FORTRAN types for these realtype sizes are:

- single – equivalent to a REAL or REAL*4 in FORTRAN

- double – equivalent to a DOUBLE PRECISION or REAL*8 in FORTRAN

- extended – equivalent to a REAL*16 in FORTRAN

5.3   FIDA routines

The user-callable functions, with the corresponding IDA functions, are as follows:

- Interface to the NVECTOR modules

    - FNVINITS (defined by NVECTOR_SERIAL) interfaces to N_VNewEmpty_Serial.
    - FNVINITP (defined by NVECTOR_PARALLEL) interfaces to N_VNewEmpty_Parallel.
    - FNVINITOMP (defined by NVECTOR_OPENMP) interfaces to N_VNewEmpty_OpenMP.
    - FNVINITPTS (defined by NVECTOR_PTHREADS) interfaces to N_VNewEmpty_Pthreads.

- Interface to the SUNMATRIX modules

    - FSUNBANDMATINIT (defined by SUNMATRIX_BAND) interfaces to SUNBandMatrix.
    - FSUNDENSEMATINIT (defined by SUNMATRIX_DENSE) interfaces to SUNDenseMatrix.
    - FSUNSPARSEMATINIT (defined by SUNMATRIX_SPARSE) interfaces to SUNSparseMatrix.

- Interface to the SUNLINSOL modules

    - FSUNBANDLINSOLINIT (defined by SUNLINSOL_BAND) interfaces to SUNLinSol_Band.
    - FSUNDENSELINSOLINIT (defined by SUNLINSOL_DENSE) interfaces to SUNLinSol_Dense.
    - FSUNKLUINIT (defined by SUNLINSOL_KLU) interfaces to SUNLinSol_KLU.
    - FSUNKLUREINIT (defined by SUNLINSOL_KLU) interfaces to SUNLinSol_KLUReinit.
    - FSUNLAPACKBANDINIT (defined by SUNLINSOL_LAPACKBAND) interfaces to SUNLinSol_LapackBand.
    - FSUNLAPACKDENSEINIT (defined by SUNLINSOL_LAPACKDENSE) interfaces to SUNLinSol_LapackDense.
    - FSUNPCGINIT (defined by SUNLINSOL_PCG) interfaces to SUNLinSol_PCG.
    - FSUNSPBCGSINIT (defined by SUNLINSOL_SPBCGS) interfaces to SUNLinSol_SPBCGS.
    - FSUNSPFGMRINIT (defined by SUNLINSOL_SPFGMR) interfaces to SUNLinSol_SPFGMR.
    - FSUNSPGMRINIT (defined by SUNLINSOL_SPGMR) interfaces to SUNLinSol_SPGMR.
    - FSUNSPTFQMRINIT (defined by SUNLINSOL_SPTFQMR) interfaces to SUNLinSol_SPTFQMR.
    - FSUNSUPERLUMTINIT (defined by SUNLINSOL_SUPERLUMT) interfaces to SUNLinSol_SuperLUMT.

-

- Interface to the main IDA module

  - FIDAMALLOC interfaces to `IDACreate`, `IDASetUserData`, `IDAInit`, `IDASStolerances`, and `IDASVtolerances`.

  - FIDAREINIT interfaces to `IDAReInit` and `IDASStolerances`/`IDASVtolerances`.

  - FIDASETIIN, FIDASETVIN, and FIDASETRIN interface to `IDASet*` functions.

  - FIDATOLREINIT interfaces to `IDASStolerances`/`IDASVtolerances`.

  - FIDACALCIC interfaces to `IDACalcIC`.

  - FIDAEWTSET interfaces to `IDAWFtolerances`.

  - FIDASOLVE interfaces to `IDASolve`, `IDAGet*` functions, and to the optional output functions for the selected linear solver module.

  - FIDAGETDKY interfaces to `IDAGetDky`.

  - FIDAGETERRWEIGHTS interfaces to `IDAGetErrWeights`.

  - FIDAGETESTLOCALERR interfaces to `IDAGetEstLocalErrors`.

  - FIDAFREE interfaces to `IDAFree`.

- Interface to the IDALS module

  - FIDALSINIT interfaces to `IDASetLinearSolver`.

  - FIDALSSETEPSLIN interfaces to `IDASetEpsLin`

  - FIDALSSETJAC interfaces to `IDASetJacTimes`.

  - FIDALSSETPREC interfaces to `IDASetPreconditioner`.

  - FIDADENSESETJAC interfaces to `IDASetJacFn`.

  - FIDABANDSETJAC interfaces to `IDASetJacFn`.

  - FIDASPARSESETJAC interfaces to `IDASetJacFn`.

The user-supplied functions, each listed with the corresponding internal interface function which calls it (and its type within IDA), are as follows:

FIDA routine (FORTRAN, user-supplied)	IDA function (C, interface)	IDA type of interface function
`FIDARESFUN`	`FIDAresfn`	`IDAResFn`
`FIDAEWT`	`FIDAEwtSet`	`IDAEwtFn`
`FIDADJAC`	`FIDADenseJac`	`IDALsJacFn`
`FIDABJAC`	`FIDABandJac`	`IDALsJacFn`
`FIDASPJAC`	`FIDASparseJac`	`IDALsJacFn`
`FIDAPSOL`	`FIDAPSol`	`IDALsPrecSolveFn`
`FIDAPSET`	`FIDAPSet`	`IDALsPrecSetupFn`
`FIDAJTIMES`	`FIDAJtimes`	`IDALsJacTimesVecFn`
`FIDAJTSETUP`	`FIDAJTSetup`	`IDALsJacTimesSetupFn`

In contrast to the case of direct use of IDA, and of most FORTRAN DAE solvers, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program.

5.4   Usage of the FIDA interface module

The usage of FIDA requires calls to a variety of interface functions, depending on the method options selected, and one or more user-supplied routines which define the problem to be solved. These function calls and user routines are summarized separately below. Some details are omitted, and the user is referred to the description of the corresponding IDA functions for information on the arguments of any given user-callable interface routine, or of a given user-supplied function called by an interface function. The usage of FIDA for rootfinding, and usage of FIDA with preconditioner modules, are each described in later sections.

1. **Residual function specification**

    The user must, in all cases, supply the following FORTRAN routine

    ```
    SUBROUTINE FIDARESFUN (T, Y, YP, R, IPAR, RPAR, IER)
    DIMENSION Y(*), YP(*), R(*), IPAR(*), RPAR(*)
    ```

    It must set the R array to $F(t, y, \dot{y})$, the residual function of the DAE system, as a function of T $= t$ and the arrays Y $= y$ and YP $= \dot{y}$. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC. It should return IER $= 0$ if it was successful, IER $= 1$ if it had a recoverable failure, or IER $= -1$ if it had a non-recoverable failure.

2. NVECTOR **module initialization**

    If using one of the NVECTOR modules supplied with SUNDIALS, the user must make a call of the form

    ```
    CALL FNVINIT***(...)
    ```

    in which the name and call sequence are as described in the appropriate section of Chapter 6.

3. SUNMATRIX **module initialization**

    In the case of a stiff system, the implicit BDF method involves the solution of linear systems related to the Jacobian of the DAE system. If using a Newton iteration with the direct SUNLINSOL linear solver module and one of the SUNMATRIX modules supplied with SUNDIALS, the user must make a call of the form

    ```
    CALL FSUN***MATINIT(...)
    ```

    in which the name and call sequence are as described in the appropriate section of Chapter 7. Note that the dense, band, or sparse matrix options are usable only in a serial or multi-threaded environment.

4. SUNLINSOL **module initialization**

    If using a Newton iteration with one of the SUNLINSOL linear solver modules supplied with SUN-DIALS, the user must make a call of the form

    ```
    CALL FSUNBANDLINSOLINIT(...)
    CALL FSUNDENSELINSOLINIT(...)
    CALL FSUNKLUINIT(...)
    CALL FSUNLAPACKBANDINIT(...)
    CALL FSUNLAPACKDENSEINIT(...)
    CALL FSUNPCGINIT(...)
    CALL FSUNSPBCGSINIT(...)
    CALL FSUNSPFGMRINIT(...)
    ```

```
CALL FSUNSPGMRINIT(...)
CALL FSUNSPTFQMRINIT(...)
CALL FSUNSUPERLUMTINIT(...)
```

in which the call sequence is as described in the appropriate section of Chapter 8. Note that the dense, band, or sparse solvers are usable only in a serial or multi-threaded environment.

Once one of these solvers has been initialized, its solver parameters may be modified using a call to the functions

```
CALL FSUNKLUSETORDERING(...)
CALL FSUNSUPERLUMTSETORDERING(...)
CALL FSUNPCGSETPRECTYPE(...)
CALL FSUNPCGSETMAXL(...)
CALL FSUNSPBCGSSETPRECTYPE(...)
CALL FSUNSPBCGSSETMAXL(...)
CALL FSUNSPFGMRSETGSTYPE(...)
CALL FSUNSPFGMRSETPRECTYPE(...)
CALL FSUNSPGMRSETGSTYPE(...)
CALL FSUNSPGMRSETPRECTYPE(...)
CALL FSUNSPTFQMRSETPRECTYPE(...)
CALL FSUNSPTFQMRSETMAXL(...)
```

where again the call sequences are described in the appropriate sections of Chapter 8.

5. **Problem specification**

To set various problem and solution parameters and allocate internal memory, make the following call:

FIDAMALLOC

Call	CALL FIDAMALLOC(T0, Y0, YP0, IATOL, RTOL, ATOL,
	& IOUT, ROUT, IPAR, RPAR, IER)
Description	This function provides required problem and solution specifications, specifies optional inputs, allocates internal memory, and initializes IDA.

Arguments

T0	is the initial value of t.
Y0	is an array of initial conditions for y.
YP0	is an array of initial conditions for $\dot{y}$.
IATOL	specifies the type for absolute tolerance ATOL: 1 for scalar or 2 for array. If IATOL= 3, the arguments RTOL and ATOL are ignored and the user is expected to subsequently call FIDAEWTSET and provide the function FIDAEWT.
RTOL	is the relative tolerance (scalar).
ATOL	is the absolute tolerance (scalar or array).
IOUT	is an integer array of length at least 21 for integer optional outputs.
ROUT	is a real array of length at least 6 for real optional outputs.
IPAR	is an integer array of user data which will be passed unmodified to all user-provided routines.
RPAR	is a real array of user data which will be passed unmodified to all user-provided routines.

Return value   IER is a return completion flag. Values are 0 for successful return and -1 otherwise. See printed message for details in case of failure.

Notes   The user integer data arrays IOUT and IPAR must be declared as INTEGER*4 or INTEGER*8 according to the C type `long int`.

Modifications to the user data arrays `IPAR` and `RPAR` inside a user-provided routine will be propagated to all subsequent calls to such routines.

The optional outputs associated with the main IDA integrator are listed in Table 5.2.

As an alternative to providing tolerances in the call to `FIDAMALLOC`, the user may provide a routine to compute the error weights used in the WRMS norm evaluations. If supplied, it must have the following form:

```
SUBROUTINE FIDAEWT (Y, EWT, IPAR, RPAR, IER)
DIMENSION Y(*), EWT(*), IPAR(*), RPAR(*)
```

It must set the positive components of the error weight vector `EWT` for the calculation of the WRMS norm of `Y`. On return, set `IER = 0` if `FIDAEWT` was successful, and nonzero otherwise. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`.

If the `FIDAEWT` routine is provided, then, following the call to `FIDAMALLOC`, the user must make the call:

```
CALL FIDAEWTSET (FLAG, IER)
```

with `FLAG` $\neq 0$ to specify use of the user-supplied error weight routine. The argument `IER` is an error return flag, which is 0 for success or non-zero if an error occurred.

6. **Set optional inputs**

   Call `FIDASETIIN`, `FIDASETRIN`, and/or `FIDASETVIN` to set desired optional inputs, if any. See §5.5 for details.

7. **Linear solver interface specification**

   The variable-order, variable-coefficient BDF method used by IDA involves the solution of linear systems related to the system Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial \dot{y}$. See Eq. (2.4). To attach the linear solver (and optionally the matrix) objects initialized in steps 3 and 4 above, the user of FIDA must initialize the IDALS linear solver interface. To attach any SUNLINSOL object (and optional SUNMATRIX object) to IDA, then following calls to initialize the SUNLINSOL (and SUNMATRIX) object(s) in steps 3 and 4 above, the user must make the call:

   ```
   CALL FIDALSINIT(IER)
   ```

   `IER` is an error return flag set on 0 on success or -1 if a memory failure occurred.

   The previous routines `FIDADLSINIT` and `FIDASPILSINIT` 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.

   IDALS **with dense Jacobian matrix**

   As an option when using the IDALS interface with the SUNLINSOL_DENSE or SUNLINSOL_LAPACKDENSE linear solvers, the user may supply a routine that computes a dense approximation of the system Jacobian J. If supplied, it must have the following form:

   ```
   SUBROUTINE FIDADJAC (NEQ, T, Y, YP, R, DJAC, CJ, EWT, H,
   &                     IPAR, RPAR, WK1, WK2, WK3, IER)
    DIMENSION Y(*), YP(*), R(*), EWT(*), DJAC(NEQ,*),
   &          IPAR(*), RPAR(*), WK1(*), WK2(*), WK3(*)
   ```

   This routine must compute the Jacobian and store it columnwise in `DJAC`. The vectors `WK1`, `WK2`, and `WK3` of length `NEQ` are provided as work space for use in `FIDADJAC`. The input arguments `T`, `Y`,

`YP`, `R`, and `CJ` are the current values of t, y, $\dot{y}$, $F(t, y, \dot{y})$, and α, respectively. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`. NOTE: The argument `NEQ` has a type consistent with C type `long int` even in the case when the LAPACK dense solver is to be used.

If the user's `FIDADJAC` uses difference quotient approximations, it may need to use the error weight array `EWT` and current stepsize `H` in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output `ROUT(6)`, passed from the calling program to this routine using `COMMON`.

If the `FIDADJAC` routine is provided, then, following the call to `FIDALSINIT` the user must make the call:

```
CALL FIDADENSESETJAC (FLAG, IER)
```

with `FLAG` $\neq 0$ to specify use of the user-supplied Jacobian approximation. The argument `IER` is an error return flag, which is 0 for success or non-zero if an error occurred.

IDALS **with band Jacobian matrix**

As an option when using the IDALS interface with the SUNLINSOL_BAND or SUNLINSOL_LAPACKBAND linear solvers, the user may supply a routine that computes a band approximation of the system Jacobian J. If supplied, it must have the following form:

```
SUBROUTINE FIDABJAC(NEQ, MU, ML, MDIM, T, Y, YP, R, CJ, BJAC,
&                    EWT, H, IPAR, RPAR, WK1, WK2, WK3, IER)
 DIMENSION Y(*), YP(*), R(*), EWT(*), BJAC(MDIM,*),
&          IPAR(*), RPAR(*), WK1(*), WK2(*), WK3(*)
```

This routine must load the `MDIM` by `NEQ` array `BJAC` with the Jacobian matrix at the current $(t, y, \dot{y})$ in band form. Store in `BJAC`(k, j) the Jacobian element $J_{i,j}$ with $k = i - j +$`MU`$+1$ ($k = 1 \cdots$ `ML` $+$ `MU` $+ 1$) and $j = 1 \cdots N$. The vectors `WK1`, `WK2`, and `WK3` of length `NEQ` are provided as work space for use in `FIDABJAC`. The input arguments `T`, `Y`, `YP`, `R`, and `CJ` are the current values of t, y, $\dot{y}$, $F(t, y, \dot{y})$, and α, respectively. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`. NOTE: The arguments `NEQ`, `MU`, `ML`, and `MDIM` have a type consistent with C type `long int` even in the case when the LAPACK band solver is to be used.

If the user's `FIDABJAC` uses difference quotient approximations, it may need to use the error weight array `EWT` and current stepsize `H` in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output `ROUT(6)`, passed from the calling program to this routine using `COMMON`.

If the `FIDABJAC` routine is provided, then, following the call to `FIDALSINIT`, the user must make the call:

```
CALL FIDABANDSETJAC (FLAG, IER)
```

with `FLAG` $\neq 0$ to specify use of the user-supplied Jacobian approximation. The argument `IER` is an error return flag, which is 0 for success or non-zero if an error occurred.

IDALS **with sparse Jacobian matrix**

When using the IDALS interface with the SUNLINSOL_KLU or SUNLINSOL_SUPERLUMT linear solvers, the user must supply the `FIDASPJAC` routine that computes a compressed-sparse-column (CSC) or compressed-sparse-row (CSR) approximation of the system Jacobian $J = \partial F / \partial y + c_j \partial F / \partial \dot{y}$. If supplied, it must have the following form:

```
SUBROUTINE FIDASPJAC(T, CJ, Y, YP, R, N, NNZ, JDATA, JINDEXVALS,
&                     JINDEXPTRS, H, IPAR, RPAR, WK1, WK2, WK3, IER)
```

It must load the N by N compressed sparse column [or compressed sparse row] matrix with storage for NNZ nonzeros, stored in the arrays JDATA (nonzero values), JINDEXVALS (row [or column] indices for each nonzero), JINDEXPTRS (indices for start of each column [or row]), with the Jacobian matrix at the current (t, y) in CSC [or CSR] form (see sunmatrix_sparse.h for more information). The arguments are T, the current time; CJ, scalar in the system proportional to the inverse step size; Y, an array containing state variables; YP, an array containing state derivatives; R, an array containing the system nonlinear residual; N, the number of matrix rows/columns in the Jacobian; NNZ, allocated length of nonzero storage; JDATA, nonzero values in the Jacobian (of length NNZ); JINDEXVALS, row [or column] indices for each nonzero in Jacobian (of length NNZ); JINDEXPTRS, pointers to each Jacobian column [or row] in the two preceding arrays (of length N+1); H, the current step size; IPAR, an array containing integer user data that was passed to FIDAMALLOC; RPAR, an array containing real user data that was passed to FIDAMALLOC; WK*, work arrays containing temporary workspace of same size as Y; and IER, error return code (0 if successful, > 0 if a recoverable error occurred, or < 0 if an unrecoverable error occurred.)

To indicate that the FIDASPJAC routine has been provided, then following the call to FIDALSINIT, the following call must be made

```
CALL FIDASPARSESETJAC (IER)
```

The int return flag IER is an error return flag which is 0 for success or nonzero for an error.

IDALS with Jacobian-vector product

As an option when using the IDALS linear solver interface, the user may supply a routine that computes the product of the system Jacobian $J = \partial F/\partial y + \alpha \partial F/\partial \dot{y}$ and a given vector v. If supplied, it must have the following form:

```
SUBROUTINE FIDAJTIMES(T, Y, YP, R, V, FJV, CJ, EWT, H,
&                      IPAR, RPAR, WK1, WK2, IER)
DIMENSION Y(*), YP(*), R(*), V(*), FJV(*), EWT(*),
&         IPAR(*), RPAR(*), WK1(*), WK2(*)
```

This routine must compute the product vector Jv, where the vector v is stored in V, and store the product in FJV. On return, set IER = 0 if FIDAJTIMES was successful, and nonzero otherwise. The vectors W1K and WK2, of length NEQ, are provided as work space for use in FIDAJTIMES. The input arguments T, Y, YP, R, and CJ are the current values of t, y, $\dot{y}$, $F(t, y, \dot{y})$, and α, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDAJTIMES uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

If the user's Jacobian-times-vector product routine requires that any Jacobian related data be evaluated or preprocessed, then the following routine can be used for the evaluation and preprocessing of this data:

```
SUBROUTINE FIDAJTSETUP (T, Y, YP, R, CJ, EWT, H, IPAR, RPAR, IER)
DIMENSION Y(*), YP(*), R(*), EWT(*), IPAR(*), RPAR(*)
```

Typically this routine will use only T, Y, and IDAYP. It should compute any necessary data for subsequent calls to FIDAJTIMES. On return, set IER = 0 if FIDAJTSETUP was successful, and nonzero otherwise. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

To indicate that the FIDAJTIMES and FIDAJTSETUP routines have been provided, then following the call to FIDALSINIT, the following call must be made

```
      CALL FIDALSSETJAC (FLAG, IER)
```

with FLAG $\neq$ 0. The return flag IER is 0 if successful, or negative if a memory error occurred.

The previous routine FIDASPILSETJAC 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.

If the user calls FIDALSSETJAC, the routine FIDAJTSETUP must be provided, even if it is not needed, and it must return IER=0.

⚠

IDALS **with preconditioning**

If user-supplied preconditioning is to be performed, the following routine must be supplied for solution of the preconditioner linear system:

```
      SUBROUTINE FIDAPSOL(T, Y, YP, R, RV, ZV, CJ, DELTA, EWT,
     &                    IPAR, RPAR, IER)
      DIMENSION Y(*), YP(*), R(*), RV(*), ZV(*), EWT(*),
     &          IPAR(*), RPAR(*)
```

It must solve the preconditioner linear system $Pz = r$, where $r = $ RV is input, and store the solution z in ZV. Here P is the left preconditioner. The input arguments T, Y, YP, R, and CJ are the current values of t, y, $\dot{y}$, $F(t, y, \dot{y})$, and α, respectively. On return, set IER = 0 if FIDAPSOL was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred.

The arguments EWT and DELTA are input and provide the error weight array and a scalar tolerance, respectively, for use by FIDAPSOL if it uses an iterative method in its solution. In that case, the residual vector $\rho = r - Pz$ of the system should be made less than DELTA in weighted ℓ_2 norm, i.e. $\sqrt{\sum(\rho_i * \text{EWT}[i])^2} < $ DELTA. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's preconditioner requires that any Jacobian-related data be evaluated or preprocessed, then the following routine is to be used for the evaluation and preprocessing of the preconditioner:

```
      SUBROUTINE FIDAPSET(T, Y, YP, R, CJ, EWT, H,
     &                    IPAR, RPAR, IER)
      DIMENSION Y(*), YP(*), R(*), EWT(*),
     &          IPAR(*), RPAR(*)
```

It must perform any evaluation of Jacobian-related data and preprocessing needed for the solution of the preconditioner linear systems by FIDAPSOL. The input arguments T, Y, YP, R, and CJ are the current values of t, y, $\dot{y}$, $F(t, y, \dot{y})$, and α, respectively. On return, set IER = 0 if FIDAPSET was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FIDAMALLOC.

If the user's FIDAPSET uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using COMMON.

To indicate that the FIDAPSET and FIDAPSOL routines are supplied, then following the call to FIDALSINIT, the user must call

```
      CALL FIDALSSETPREC (FLAG, IER)
```

with `FLAG` $\neq$ 0. The return flag `IER` is 0 if successful, or negative if a memory error occurred. In addition, the user must supply preconditioner routines `FIDAPSET` and `FIDAPSOL`.

The previous routine `FIDASPILSETPREC` 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.

If the user calls `FIDALSSETPREC`, the subroutine `FIDAPSET` must be provided, even if it is not needed, and it must return `IER = 0`.

8. **Correct initial values**

   Optionally, to correct the initial values y and/or $\dot{y}$, make the call

   ```
   CALL FIDACALCIC (ICOPT, TOUT1, IER)
   ```

   (See §2.1 for details.) The arguments are as follows: `ICOPT` is 1 for initializing the algebraic components of y and differential components of $\dot{y}$, or 2 for initializing all of y. `IER` is an error return flag, which is 0 for success, or negative for a failure (see `IDACalcIC` return values).

9. **Problem solution**

   Carrying out the integration is accomplished by making calls as follows:

   ```
   CALL FIDASOLVE (TOUT, T, Y, YP, ITASK, IER)
   ```

   The arguments are as follows. `TOUT` specifies the next value of t at which a solution is desired (input). `T` is the value of t reached by the solver on output. `Y` is an array containing the computed solution vector y on output. `YP` is an array containing the computed solution vector $\dot{y}$ on output. `ITASK` is a task indicator and should be set to 1 for normal mode (overshoot `TOUT` and interpolate), or to 2 for one-step mode (return after each internal step taken). `IER` is a completion flag and will be set to a positive value upon successful return or to a negative value if an error occurred. These values correspond to the `IDASolve` returns (see §4.5.7 and §B.2). The current values of the optional outputs are available in `IOUT` and `ROUT` (see Table 5.2).

10. **Additional solution output**

    After a successful return from `FIDASOLVE`, the routine `FIDAGETDKY` may be called to get interpolated values of y or any derivative $d^k y/dt^k$ for k not exceeding the current method order, and for any value of t in the last internal step taken by IDA. The call is as follows:

    ```
    CALL FIDAGETDKY (T, K, DKY, IER)
    ```

    where `T` is the input value of t at which solution derivative is desired, `K` is the derivative order, and `DKY` is an array containing the computed vector $y^{(K)}(t)$ on return. The value of `T` must lie between `TCUR - HLAST` and `TCUR`. The value of `K` must satisfy $0 \leq K \leq$ `QLAST`. (See the optional outputs for `TCUR`, `HLAST`, and `QLAST`.) The return flag `IER` is set to 0 upon successful return, or to a negative value to indicate an illegal input.

11. **Problem reinitialization**

    To re-initialize the IDA solver for the solution of a new problem of the same size as one already solved, make the following call:

    ```
    CALL FIDAREINIT (T0, Y0, YP0, IATOL, RTOL, ATOL, IER)
    ```

    The arguments have the same names and meanings as those of `FIDAMALLOC`. `FIDAREINIT` performs the same initializations as `FIDAMALLOC`, but does no memory allocation, using instead the existing internal memory created by the previous `FIDAMALLOC` call.

Following this call, if the choice of linear solver is being changed then a user must make a call to create the alternate SUNLINSOL module and then attach it to the IDALS interface, as shown above. If only linear solver parameters are being modified, then these calls may be made without re-attaching to the IDALS interface.

12. **Memory deallocation**

To free the internal memory created by the call to `FIDAMALLOC`, `FIDALSINIT`, `FNVINIT*` and `FSUN***MATINIT`, make the call

```
CALL FIDAFREE
```

5.5   FIDA optional input and output

In order to keep the number of user-callable FIDA interface routines to a minimum, optional inputs to the IDA solver are passed through only three routines: `FIDASETIIN` for integer optional inputs, `FIDASETRIN` for real optional inputs, and `FIDASETVIN` for real vector (array) optional inputs. These functions should be called as follows:

```
CALL FIDASETIIN(KEY, IVAL, IER)
CALL FIDASETRIN(KEY, RVAL, IER)
CALL FIDASETVIN(KEY, VVAL, IER)
```

where `KEY` is a quoted string indicating which optional input is set (see Table 5.1), `IVAL` is the input integer value, `RVAL` is the input real value (scalar), `VVAL` is the input real array, and `IER` is an integer return flag which is set to 0 on success and a negative value if a failure occurred. `IVAL` should be declared so as to match C type `long int`.

When using `FIDASETVIN` to specify the variable types (`KEY = 'ID_VEC'`) the components in the array `VVAL` must be 1.0 to indicate a differential variable, or 0.0 to indicate an algebraic variable. Note that this array is required only if `FIDACALCIC` is to be called with `ICOPT = 1`, or if algebraic variables are suppressed from the error test (indicated using `FIDASETIIN` with `KEY = 'SUPPRESS_ALG'`). When using `FIDASETVIN` to specify optional constraints on the solution vector (`KEY = 'CONSTR_VEC'`) the components in the array `VVAL` should be one of -2.0, -1.0, 0.0, 1.0, or 2.0. See the description of `IDASetConstraints` (§4.5.8.1) for details.

The optional outputs from the IDA solver are accessed not through individual functions, but rather through a pair of arrays, `IOUT` (integer type) of dimension at least 21, and `ROUT` (real type) of dimension at least 6. These arrays are owned (and allocated) by the user and are passed as arguments to `FIDAMALLOC`. Table 5.2 lists the entries in these two arrays and specifies the optional variable as well as the IDA function which is actually called to extract the optional output.

For more details on the optional inputs and outputs, see §4.5.8 and §4.5.10.

In addition to the optional inputs communicated through `FIDASET*` calls and the optional outputs extracted from `IOUT` and `ROUT`, the following user-callable routines are available:

To reset the tolerances at any time, make the following call:

```
CALL FIDATOLREINIT (IATOL, RTOL, ATOL, IER)
```

The tolerance arguments have the same names and meanings as those of `FIDAMALLOC`. The error return flag `IER` is 0 if successful, and negative if there was a memory failure or illegal input.

To obtain the error weight array `EWT`, containing the multiplicative error weights used the WRMS norms, make the following call:

```
CALL FIDAGETERRWEIGHTS (EWT, IER)
```

This computes the `EWT` array, normally defined by Eq. (2.6). The array `EWT`, of length `NEQ` or `NLOCAL`, must already have been declared by the user. The error return flag `IER` is zero if successful, and negative if there was a memory error.

Table 5.1: Keys for setting FIDA optional inputs

Integer optional inputs (`FIDASETIIN`)

Key	Optional input	Default value
MAX_ORD	Maximum LMM method order	5
MAX_NSTEPS	Maximum no. of internal steps before t_{out}	500
MAX_ERRFAIL	Maximum no. of error test failures	10
MAX_NITERS	Maximum no. of nonlinear iterations	4
MAX_CONVFAIL	Maximum no. of convergence failures	10
SUPPRESS_ALG	Suppress alg. vars. from error test (1 = SUNTRUE)	0 (= SUNFALSE)
MAX_NSTEPS_IC	Maximum no. of steps for IC calc.	5
MAX_NITERS_IC	Maximum no. of Newton iterations for IC calc.	10
MAX_NJE_IC	Maximum no. of Jac. evals fo IC calc.	4
LS_OFF_IC	Turn off line search (1 = SUNTRUE)	0 (= SUNFALSE)

Real optional inputs (`FIDASETRIN`)

Key	Optional input	Default value
INIT_STEP	Initial step size	estimated
MAX_STEP	Maximum absolute step size	∞
STOP_TIME	Value of t_{stop}	undefined
NLCONV_COEF	Coeff. in the nonlinear conv. test	0.33
NLCONV_COEF_IC	Coeff. in the nonlinear conv. test for IC calc.	0.0033
STEP_TOL_IC	Lower bound on Newton step for IC calc.	uround$^{2/3}$

Real vector optional inputs (`FIDASETVIN`)

Key	Optional input	Default value
ID_VEC	Differential/algebraic component types	undefined
CONSTR_VEC	Inequality constraints on solution	undefined

Table 5.2: Description of the FIDA optional output arrays IOUT and ROUT

Integer output array IOUT

Index	Optional output	IDA function
IDA main solver		
1	LENRW	IDAGetWorkSpace
2	LENIW	IDAGetWorkSpace
3	NST	IDAGetNumSteps
4	NRE	IDAGetNumResEvals
5	NETF	IDAGetNumErrTestFails
6	NNCFAILS	IDAGetNonlinSolvConvFails
7	NNI	IDAGetNumNonlinSolvIters
8	NSETUPS	IDAGetNumLinSolvSetups
9	QLAST	IDAGetLastOrder
10	QCUR	IDAGetCurrentOrder
11	NBCKTRKOPS	IDAGetNumBacktrackOps
12	NGE	IDAGetNumGEvals
IDALS linear solver interface		
13	LENRWLS	IDAGetLinWorkSpace
14	LENIWLS	IDAGetLinWorkSpace
15	LS_FLAG	IDAGetLastLinFlag
16	NRELS	IDAGetNumLinResEvals
17	NJE	IDAGetNumJacEvals
18	NJTS	IDAGetNumJTSetupEvals
19	NJT	IDAGetNumJtimesEvals
20	NPE	IDAGetNumPrecEvals
21	NPS	IDAGetNumPrecSolves
22	NLI	IDAGetNumLinIters
23	NCFL	IDAGetNumLinConvFails

Real output array ROUT

Index	Optional output	IDA function
1	H0_USED	IDAGetActualInitStep
2	HLAST	IDAGetLastStep
3	HCUR	IDAGetCurrentStep
4	TCUR	IDAGetCurrentTime
5	TOLFACT	IDAGetTolScaleFactor
6	UROUND	unit roundoff

To obtain the estimated local errors, following a successful call to `FIDASOLVE`, make the following call:

```
CALL FIDAGETESTLOCALERR (ELE, IER)
```

This computes the `ELE` array of estimated local errors as of the last step taken. The array `ELE` must already have been declared by the user. The error return flag `IER` is zero if successful, and negative if there was a memory error.

5.6 Usage of the FIDAROOT interface to rootfinding

The FIDAROOT interface package allows programs written in FORTRAN to use the rootfinding feature of the IDA solver module. The user-callable functions in FIDAROOT, with the corresponding IDA functions, are as follows:

- `FIDAROOTINIT` interfaces to `IDARootInit`.

- `FIDAROOTINFO` interfaces to `IDAGetRootInfo`.

- `FIDAROOTFREE` interfaces to `IDARootFree`.

Note that, at this time FIDAROOT does not provide support to specify the direction of zero-crossing that is to be monitored. Instead, all roots are considered. However, the actual direction of zero-crossing is reported (through the sign of the non-zero elements in the array `INFO` returned by `FIDAROTINFO`).

In order to use the rootfinding feature of IDA, the following call must be made, after calling `FIDAMALLOC` but prior to calling `FIDASOLVE`, to allocate and initialize memory for the `FIDAROOT` module:

```
CALL FIDAROOTINIT (NRTFN, IER)
```

The arguments are as follows: `NRTFN` is the number of root functions. `IER` is a return completion flag; its values are 0 for success, -1 if the `IDA` memory was `NULL`, and -14 if a memory allocation failed.

To specifiy the functions whose roots are to be found, the user must define the following routine:

```
SUBROUTINE FIDAROOTFN (T, Y, YP, G, IPAR, RPAR, IER)
DIMENSION Y(*), YP(*), G(*), IPAR(*), RPAR(*)
```

It must set the `G` array, of length `NRTFN`, with components $g_i(t, y, \dot{y})$, as a function of `T` $= t$ and the arrays `Y` $= y$ and `YP` $= \dot{y}$. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`. Set `IER` on 0 if successful, or on a non-zero value if an error occurred.

When making calls to `FIDASOLVE` to solve the DAE system, the occurrence of a root is flagged by the return value `IER` $= 2$. In that case, if `NRTFN` > 1, the functions g_i which were found to have a root can be identified by making the following call:

```
CALL FIDAROOTINFO (NRTFN, INFO, IER)
```

The arguments are as follows: `NRTFN` is the number of root functions. `INFO` is an integer array of length `NRTFN` with root information. `IER` is a return completion flag; its values are 0 for success, negative if there was a memory failure. The returned values of `INFO(i)` (i= 1,..., `NRTFN`) are 0 or ±1, such that `INFO(i)` $= +1$ if $g_\mathtt{i}$ was found to have a root and $g_\mathtt{i}$ is increasing, `INFO(i)` $= -1$ if $g_\mathtt{i}$ was found to have a root and $g_\mathtt{i}$ is dereasing, and `INFO(i)` $= 0$ otherwise.

The total number of calls made to the root function `FIDAROOTFN`, denoted `NGE`, can be obtained from `IOUT(12)`. If the FIDA/IDA memory block is reinitialized to solve a different problem via a call to `FIDAREINIT`, then the counter `NGE` is reset to zero.

To free the memory resources allocated by a prior call to `FIDAROOTINIT`, make the following call:

```
CALL FIDAROOTFREE
```

See §4.5.6 for additional information on the rootfinding feature.

5.7 Usage of the FIDABBD interface to IDABBDPRE

The FIDABBD interface sub-module is a package of C functions which, as part of the FIDA interface module, support the use of the IDA solver with the parallel NVECTOR_PARALLEL module, in a combination of any of the Krylov iterative solver modules with the IDABBDPRE preconditioner module (see §4.7).

The user-callable functions in this package, with the corresponding IDA and IDABBDPRE functions, are as follows:

- `FIDABBDINIT` interfaces to `IDABBDPrecAlloc`.

- `FIDABBDREINIT` interfaces to `IDABBDPrecReInit`.

- `FIDABBDOPT` interfaces to IDABBDPRE optional output functions.

- `FIDABBDFREE` interfaces to `IDABBDPrecFree`.

In addition to the FORTRAN residual function `FIDARESFUN`, the user-supplied functions used by this package, are listed below, each with the corresponding interface function which calls it (and its type within IDABBDPRE or IDA):

FIDABBD routine (FORTRAN)	IDA function (C)	IDA function type
FIDAGLOCFN	FIDAgloc	IDABBDLocalFn
FIDACOMMFN	FIDAcfn	IDABBDCommFn
FIDAJTIMES	FIDAJtimes	IDALsJacTimesVecFn
FIDAJTSETUP	FIDAJTSetup	IDALsJacTimesSetupFn

As with the rest of the FIDA routines, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program. Additionally, based on flags discussed above in §5.3, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fidabbd.h`.

The following is a summary of the usage of this module. Steps that are unchanged from the main program described in §5.4 are grayed-out.

1. **Residual function specification**

2. NVECTOR **module initialization**

3. SUNLINSOL **module initialization**

   Initialize one of the iterative SUNLINSOL modules, by calling one of `FSUNPCGINIT`, `FSUNSPBCGSINIT`, `FSUNSPFGMRINIT`, `FSUNSPGMRINIT` or `FSUNSPTFQMRINIT`.

4. **Problem specification**

5. **Set optional inputs**

6. **Linear solver interface specification**

   Initialize the IDALS iterative linear solver interface by calling `FIDALSINIT`.

7. **BBD preconditioner initialization**

   To initialize the IDABBDPRE preconditioner, make the following call:

   ```
   CALL FIDABBDINIT (NLOCAL, MUDQ, MLDQ, MU, ML, DQRELY, IER)
   ```

   The arguments are as follows. `NLOCAL` is the local size of vectors on this processor. `MUDQ` and `MLDQ` are the upper and lower half-bandwidths to be used in the computation of the local Jacobian blocks by difference quotients. These may be smaller than the true half-bandwidths of the Jacobian of

the local block of G, when smaller values may provide greater efficiency. `MU` and `ML` are the upper and lower half-bandwidths of the band matrix that is retained as an approximation of the local Jacobian block. These may be smaller than `MUDQ` and `MLDQ`. `DQRELY` is the relative increment factor in y for difference quotients (optional). A value of 0.0 indicates the default, $\sqrt{\text{unit roundoff}}$. `IER` is a return completion flag. A value of 0 indicates success, while a value of -1 indicates that a memory failure occurred or that an input had an illegal value.

8. **Correct initial values**

9. **Problem solution**

10. **Additional solution output**

11. IDABBDPRE **Optional outputs**

    Optional outputs specific to the SPGMR, SPBCGS, or SPTFQMR solver are listed in Table 5.2. To obtain the optional outputs associated with the IDABBDPRE module, make the following call:

        CALL FIDABBDOPT (LENRWBBD, LENIWBBD, NGEBBD)

    The arguments should be consistent with C type `long int`. Their returned values are as follows: `LENRWBBD` is the length of real preconditioner work space, in `realtype` words. `LENIWBBD` is the length of integer preconditioner work space, in integer words. Both of these sizes are local to the current processor. `NGEBBD` is the number of $G(t, y, \dot{y})$ evaluations (calls to `FIDALOCFN`) so far.

12. **Problem reinitialization**

    If a sequence of problems of the same size is being solved using the same linear solver in combination with the IDABBDPRE preconditioner, then the IDA package can be re-initialized for the second and subsequent problems by calling `FIDAREINIT`, following which a call to `FIDABBDINIT` may or may not be needed. If the input arguments are the same, no `FIDABBDINIT` call is needed. If there is a change in input arguments other than `MU` or `ML`, then the user program should make the call

        CALL FIDABBDREINIT (NLOCAL, MUDQ, MLDQ, DQRELY, IER)

    This reinitializes the IDABBDPRE preconditioner, but without reallocating its memory. The arguments of the `FIDABBDREINIT` routine have the same names and meanings as those of `FIDABBDINIT`. If the value of `MU` or `ML` is being changed, then a call to `FIDABBDINIT` must be made. Finally, if there is a change in any of the linear solver inputs, then a call to one of `FSUN****INIT`, followed by a call to `FIDALSINIT` must also be made; in this case the linear solver memory is reallocated.

13. **Memory deallocation**

    (The memory allocated for the FIDABBD module is deallocated automatically by `FIDAFREE`.)

14. **User-supplied routines**

    The following two routines must be supplied for use with the IDABBDPRE module:

        SUBROUTINE FIDAGLOCFN (NLOC, T, YLOC, YPLOC, GLOC, IPAR, RPAR, IER)
        DIMENSION YLOC(*), YPLOC(*), GLOC(*), IPAR(*), RPAR(*)

    This routine is to evaluate the function $G(t, y, \dot{y})$ approximating F (possibly identical to F), in terms of $T = t$, and the arrays `YLOC` and `YPLOC` (of length `NLOC`), which are the sub-vectors of y and $\dot{y}$ local to this processor. The resulting (local) sub-vector is to be stored in the array `GLOC`. `IER` is a return flag that should be set to 0 if successful, to 1 (for a recoverable error), or to -1 (for a non-recoverable error). The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`.

```
SUBROUTINE FIDACOMMFN (NLOC, T, YLOC, YPLOC, IPAR, RPAR, IER)
DIMENSION YLOC(*), YPLOC(*), IPAR(*), RPAR(*)
```

This routine is to perform the inter-processor communication necessary for the `FIDAGLOCFN` routine. Each call to `FIDACOMMFN` is preceded by a call to the residual routine `FIDARESFUN` with the same arguments `T`, `YLOC`, and `YPLOC`. Thus `FIDACOMMFN` can omit any communications done by `FIDARESFUN` if relevant to the evaluation of `GLOC`. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FIDAMALLOC`. `IER` is a return flag that should be set to 0 if successful, to 1 (for a recoverable error), or to -1 (for a non-recoverable error).

The subroutine `FIDACOMMFN` must be supplied even if it is empty, and it must return `IER = 0`.

Optionally, the user can supply routines `FIDAJTIMES` and `FIDAJTSETUP` for the evaluation of Jacobian-vector products, as described above in step 7 in §5.4.

Chapter 6

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*        (*nvgetcommunicator)(N_Vector);
  sunindextype (*nvgetlength)(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*);
realtype     (*nvdotprodlocal)(N_Vector, N_Vector);
realtype     (*nvmaxnormlocal)(N_Vector);
realtype     (*nvminlocal)(N_Vector);
realtype     (*nvl1normlocal)(N_Vector);
booleantype  (*nvinvtestlocal)(N_Vector, N_Vector);
booleantype  (*nvconstrmasklocal)(N_Vector, N_Vector, N_Vector);
realtype     (*nvminquotientlocal)(N_Vector, N_Vector);
realtype     (*nvwsqrsumlocal)(N_Vector, N_Vector);
realtype     (*nvwsqrsummasklocal(N_Vector, 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 6.2 contains a complete list of all standard vector operations defined by the generic NVECTOR module. Tables 6.3, 6.4 and 6.5 list *optional* fused, vector array and local reduction 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. In all SUNDIALS-provided NVECTOR implementations, all fused and

vector array operations are disabled by default. However, these implementations provide 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.

Local reduction operations are similarly intended to reduce parallel communication on distributed memory systems, particularly when NVECTOR objects are combined together within a NVECTOR_MANYVECTOR object (see Section 6.12). If a particular NVECTOR implementation defines a local reduction operation as NULL, the NVECTOR_MANYVECTOR module will automatically call standard vector reduction operations as necessary to complete the desired operation. All SUNDIALS-provided NVECTOR implementations include these local reduction operations, which may be used as templates for user-defined NVECTOR implementations.

Finally, note that the generic NVECTOR module defines the functions N_VCloneVectorArray and N_VCloneVectorArrayEmpty. Both functions create (by cloning) an array of count variables of type N_Vector, each of the same type as an existing N_Vector. Their prototypes are

```
N_Vector *N_VCloneVectorArray(int count, N_Vector w);
N_Vector *N_VCloneVectorArrayEmpty(int count, N_Vector w);
```

and their definitions are based on the implementation-specific N_VClone and N_VCloneEmpty operations, respectively.

An array of variables of type N_Vector can be destroyed by calling N_VDestroyVectorArray, whose prototype is

```
void N_VDestroyVectorArray(N_Vector *vs, int count);
```

and whose definition is based on the implementation-specific N_VDestroy operation.

A particular implementation of the NVECTOR module must:

- Specify the *content* field of N_Vector.

- Define and implement the vector operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one NVECTOR module (each with different N_Vector internal data representations) in the same code.

- Define and implement user-callable constructor and destructor routines to create and free an N_Vector with the new *content* field and with *ops* pointing to the new vector operations.

- Optionally, define and implement additional user-callable routines acting on the newly defined N_Vector (e.g., a routine to print the content for debugging purposes).

- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the *content* field of the newly defined N_Vector.

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 6.1. It is recommended that a user-supplied NVECTOR implementation use the SUNDIALS_NVEC_CUSTOM identifier.

Table 6.1: 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_CUDA	CUDA parallel vector	6
SUNDIALS_NVEC_RAJA	RAJA parallel vector	7
SUNDIALS_NVEC_OPENMPDEV	OpenMP parallel vector with device offloading	8
SUNDIALS_NVEC_TRILINOS	Trilinos Tpetra vector	9
SUNDIALS_NVEC_MANYVECTOR	"ManyVector" vector	10
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	11

Table 6.2: 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 6.1.
N_VClone	`v = N_VClone(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not copy the vector, but rather allocates storage for the new vector.
N_VCloneEmpty	`v = N_VCloneEmpty(w);` Creates a new `N_Vector` of the same type as an existing vector `w` and sets the *ops* field. It does not allocate storage for data.
N_VDestroy	`N_VDestroy(v);` Destroys the `N_Vector` `v` and frees memory allocated for its internal data.
N_VSpace	`N_VSpace(nvSpec, &lrw, &liw);` Returns storage requirements for one `N_Vector`. `lrw` contains the number of realtype words and `liw` contains the number of integer words. This function is advisory only, for use in determining a user's total space requirements; it could be a dummy function in a user-supplied NVECTOR module if that information is not of interest.

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Name	**Usage and Description**
N_VGetArrayPointer	vdata = N_VGetArrayPointer(v); Returns a pointer to a `realtype` array from the N_Vector v. Note that this assumes that the internal data in N_Vector is a contiguous array of `realtype`. This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, the sparse linear solvers (serial and threaded), and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS.
N_VSetArrayPointer	N_VSetArrayPointer(vdata, v); Overwrites the data in an N_Vector with a given array of `realtype`. Note that this assumes that the internal data in N_Vector is a contiguous array of `realtype`. This routine is only used in the interfaces to the dense (serial) linear solver, hence need not exist in a user-supplied NVECTOR module for a parallel environment.
N_VGetCommunicator	N_VGetCommunicator(v); Returns a pointer to the MPI_Comm object associated with the vector (if applicable). For MPI-unaware vector implementations, this should return NULL.
N_VGetLength	N_VGetLength(v); Returns the global length (number of 'active' entries) in the NVECTOR v. This value should be cumulative across all processes if the vector is used in a parallel environment. If v contains additional storage, e.g., for parallel communication, those entries should not be included.
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.
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Name	Usage and Description
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: $y_i = |x_i|$, $i = 0, \ldots, n-1$.
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: $m = \max_i |x_i|$.
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: $m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}$.

Name	Usage and Description
N_VL1Norm	`m = N_VL1Norm(x);` Returns the ℓ_1 norm of the N_Vector x: $m = \sum_{i=0}^{n-1} |x_i|$.
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 $|x_i| \geq c$ 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.
N_VMinQuotient	`minq = N_VMinQuotient(num, denom);` This routine returns the minimum of the quotients obtained by term-wise dividing num_i by $denom_i$. 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 6.3: 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.
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.

continued from last page	
Name	**Usage and Description**

Table 6.4: Description of the NVECTOR vector array operations

Name	Usage and Description
`N_VLinearSumVectorArray`	`ier = N_VLinearSumVectorArray(nv, a, X, b, Y, Z);` This routine computes 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.
`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.
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Name	**Usage and Description**
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: $$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i})^2 \right)^{1/2}, \quad j = 0, \dots, n_v - 1,$$ 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: $$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i} H(id_i))^2 \right)^{1/2}, \quad j = 0, \dots, n_v - 1,$$ $H(id_i) = 1$ 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.
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.
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Name	**Usage and Description**
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: $$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$ 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.

Table 6.5: Description of the NVECTOR local reduction operations

Name	**Usage and Description**
N_VDotProdLocal	`d = N_VDotProdLocal(x, y);` This routine computes the MPI task-local portion of the ordinary dot product of `x` and `y`: $$d = \sum_{i=0}^{n_{local}-1} x_i y_i,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
N_VMaxNormLocal	`m = N_VMaxNormLocal(x);` This routine computes the MPI task-local portion of the maximum norm of the `N_Vector` x: $$m = \max_{0 \le i < n_{local}} |x_i|,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
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Name	**Usage and Description**
N_VMinLocal	`m = N_VMinLocal(x);` This routine computes the smallest element of the MPI task-local portion of the `N_Vector` x: $$m = \min_{0 \le i < n_{local}} x_i,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
N_VL1NormLocal	`n = N_VL1NormLocal(x);` This routine computes the MPI task-local portion of the ℓ_1 norm of the `N_Vector` x: $$n = \sum_{i=0}^{n_{local}-1} |x_i|,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
N_VWSqrSumLocal	`s = N_VWSqrSumLocal(x,w);` This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector` x with weight vector w: $$s = \sum_{i=0}^{n_{local}-1} (x_i w_i)^2,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
N_VWSqrSumMaskLocal	`s = N_VWSqrSumMaskLocal(x,w,id);` This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector` x with weight vector w built using only the elements of x corresponding to positive elements of the `N_Vector` id: $$m = \sum_{i=0}^{n_{local}-1} (x_i w_i H(id_i))^2, \quad \text{where} \quad H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \le 0 \end{cases}$$ and n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).
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Name	**Usage and Description**
N_VInvTestLocal	`t = N_VInvTestLocal(x);` Sets the MPI task-local components of the N_Vector z to be the inverses of the components of the N_Vector x, with prior testing for zero values: $$z_i = 1.0/x_i,\ i = 0,\dots,n_{local} - 1,$$ where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications). This routine returns a boolean assigned to SUNTRUE if all task-local components of x are nonzero (successful inversion) and returns SUNFALSE otherwise.
N_VConstrMaskLocal	`t = N_VConstrMaskLocal(c,x,m);` Performs the following constraint tests: $$\begin{aligned} x_i > 0 \quad &\text{if} \quad c_i = 2, \\ x_i \geq 0 \quad &\text{if} \quad c_i = 1, \\ x_i \leq 0 \quad &\text{if} \quad c_i = -1, \\ x_i < 0 \quad &\text{if} \quad c_i = -2, \text{and} \\ \text{no test} \quad &\text{if} \quad c_i = 0, \end{aligned}$$ for all MPI task-local components of the vectors. This routine returns a boolean assigned to SUNFALSE if any task-local 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.
N_VMinQuotientLocal	`minq = N_VMinQuotientLocal(num,denom);` This routine returns the minimum of the quotients obtained by term-wise dividing num_i by $denom_i$, for all MPI task-local components of the vectors. 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.

6.1 NVECTOR functions used by IDA

In Table 6.6 below, we list the vector functions used in the NVECTOR module used by the IDA package. The table also shows, for each function, which of the code modules uses the function. The IDA column shows function usage within the main integrator module, while the remaining columns show function usage within the IDALS linear solvers interface, the IDABBDPRE preconditioner module, and the FIDA module.

At this point, we should emphasize that the IDA user does not need to know anything about the usage of vector functions by the IDA code modules in order to use IDA. 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 IDA modules for user feedback.

Table 6.6: List of vector functions usage by IDA code modules

	IDA	IDALS	IDABBDPRE	FIDA
N_VGetVectorID				
N_VClone	✓	✓	✓	✓
N_VCloneEmpty		1		✓
N_VDestroy	✓	✓	✓	✓
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	✓			

3. The optional function N_VDotProdMulti is only used when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR. The remaining operations from Tables 6.3 and 6.4 not listed above are unused and a user-supplied NVECTOR module for IDA could omit these operations.

Of the functions listed in Table 6.2, N_VWL2Norm, N_VL1Norm, N_VInvTest, N_VGetCommunicator, and N_VGetLength are *not* used by IDA. Therefore a user-supplied NVECTOR module for IDA could omit these functions.

6.2 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.

6.2.1   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] )
  ```

6.2.2   NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 6.2, 6.3, 6.4 and 6.5. Their names are obtained from those in these tables by appending the suffix _Serial (e.g. N_VDestroy_Serial). All the standard vector operations listed in 6.2 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_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 op-
              eration 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 at-
  tempt 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.

6.2.3 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.

6.3 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.

6.3.1 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] )
  ```

6.3.2   NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5. Their names are obtained from those in these tables 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_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 oper-
               ations 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.

6.3.3   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.

6.4 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`.

6.4.1 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] )
  ```

6.4.2   NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5. Their names are obtained from those in these tables by appending the suffix _OpenMP (e.g. N_VDestroy_OpenMP). All the standard vector operations listed in 6.2 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_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.

6.4.3   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.

6.5   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).

```
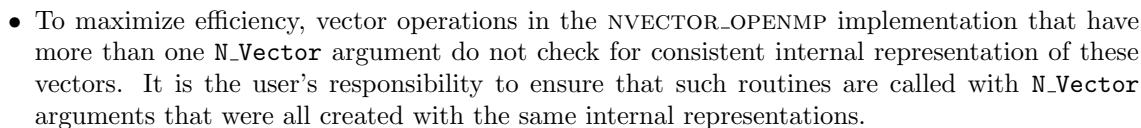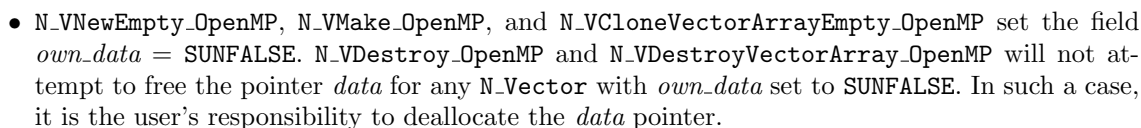struct _N_VectorContent_Pthreads {
  sunindextype length;
  booleantype own_data;
  realtype *data;
  int num_threads;
};
```

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.

6.5.1 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] )
  ```

6.5.2   NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5. Their names are obtained from those in these tables by appending the suffix _Pthreads (e.g. N_VDestroy_Pthreads). All the standard vector operations listed in 6.2 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`.

$\boxed{\texttt{N\_VPrint\_Pthreads}}$

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.

$\boxed{\texttt{N\_VPrintFile\_Pthreads}}$

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.

$\boxed{\texttt{N\_VEnableFusedOps\_Pthreads}}$

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`.

$\boxed{\texttt{N\_VEnableLinearCombination\_Pthreads}}$

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`.

$\boxed{\texttt{N\_VEnableScaleAddMulti\_Pthreads}}$

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`.

$\boxed{\texttt{N\_VEnableDotProdMulti\_Pthreads}}$

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`.

$\boxed{\texttt{N\_VEnableLinearSumVectorArray\_Pthreads}}$

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.

6.5.3 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.

6.6 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.

6.6.1   NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5, 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 [28] and the `ark_diurnal_kry_ph.c` example program for ARKODE [35].

   The names of parhyp methods are obtained from those in Tables 6.2, 6.3, 6.4, and 6.5 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.

6.7 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.

6.7.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5, 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 [27].

The names of vector operations are obtained from those in Tables 6.2, 6.3, 6.4, and 6.5 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 oper-
             ations 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 op-
               eration 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.

6.8   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.

6.8.1 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_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 6.2, 6.3, 6.4 and 6.5, 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 [28].

The names of vector operations are obtained from those in Tables 6.2, 6.3, 6.4, and 6.5 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. Addi-
              tionally, if manually instantiating the stream and reduce `ThreadPartitioning` *of a*
              `suncudavec::Vector`, *ensure that they use the same CUDA stream.*

| `N_VCopyToDevice_Cuda` |

Prototype   `void N_VCopyToDevice_Cuda(N_Vector v)`

Description   This function copies host vector data to the device.

| `N_VCopyFromDevice_Cuda` |

Prototype   `void 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 op-
              erations 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.

6.9   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.

6.9.1 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_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 6.2, 6.3, 6.4, and 6.5, 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 [28].

The names of vector operations are obtained from those in Tables 6.2, 6.3, 6.4, and 6.5 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.

6.10   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.

6.10.1   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 NVEC-TOR_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 )`

6.10.2   NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5, 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 6.2, 6.3, 6.4, and 6.5 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_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.

6.11   The NVECTOR_TRILINOS implementation

The NVECTOR_TRILINOS module is an NVECTOR wrapper around the Trilinos Tpetra vector. The interface to Tpetra is implemented in the Sundials::TpetraVectorInterface class. This class simply stores a reference counting pointer to a Tpetra vector and inherits from an empty structure

```
struct _N_VectorContent_Trilinos {};
```

to interface the C++ class with the NVECTOR C code. A pointer to an instance of this class is kept in the content field of the N_Vector object, to ensure that the Tpetra vector is not deleted for as long as the N_Vector object exists.

The Tpetra vector type in the Sundials::TpetraVectorInterface class is defined as:

```
typedef Tpetra::Vector<realtype, sunindextype, sunindextype> vector_type;
```

The Tpetra vector will use the SUNDIALS-specified realtype as its scalar type, and it will use sunindextype as the global and the local ordinal types. This type definition will use Tpetra's default node type. Available Kokkos node types in Trilinos 12.14 release are serial (single thread), OpenMP, Pthread, and CUDA. The default node type is selected when building the Kokkos package. For example, the Tpetra vector will use a CUDA node if Tpetra was built with CUDA support and the CUDA node was selected as the default when Tpetra was built.

The header file to include when using this module is nvector_trilinos.h. The installed module library to link to is libsundials_nvectrilinos.*lib* where .*lib* is typically .so for shared libraries and .a for static libraries.

6.11.1   NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in Tables 6.2, 6.5, and 6.5, except for N_VGetArrayPointer and N_VSetArrayPointer. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. When access to raw vector data is needed, it is recommended to extract the Trilinos Tpetra vector first, and then use Tpetra vector methods to access the data. Usage examples of NVECTOR_TRILINOS are provided in example programs for IDA [27].

The names of vector operations are obtained from those in Tables 6.2, 6.5, and 6.5 by appending the suffix _Trilinos (e.g. N_VDestroy_Trilinos). Vector operations call existing Tpetra::Vector methods when available. Vector operations specific to SUNDIALS are implemented as standalone functions in the namespace Sundials::TpetraVector, located in the file SundialsTpetraVectorKernels.hpp. The module NVECTOR_TRILINOS provides the following additional user-callable functions:

- N_VGetVector_Trilinos

  This C++ function takes an N_Vector as the argument and returns a reference counting pointer to the underlying Tpetra vector. This is a standalone function defined in the global namespace.

```
Teuchos::RCP<vector_type> N_VGetVector_Trilinos(N_Vector v);
```

- N_VMake_Trilinos

  This C++ function creates and allocates memory for an NVECTOR_TRILINOS wrapper around a
  user-provided Tpetra vector. This is a standalone function defined in the global namespace.

  ```
  N_Vector N_VMake_Trilinos(Teuchos::RCP<vector_type> v);
  ```

Notes

- The template parameter vector_type should be set as:
    typedef Sundials::TpetraVectorInterface::vector_type vector_type
  This will ensure that data types used in Tpetra vector match those in SUNDIALS.

- When there is a need to access components of an N_Vector_Trilinos, v, it is recommeded
  to extract the Trilinos vector object via x_vec = N_VGetVector_Trilinos(v) and then access
  components using the appropriate Trilinos functions.

- The functions N_VDestroy_Trilinos and N_VDestroyVectorArray_Trilinos only delete the
  N_Vector wrapper. The underlying Tpetra vector object will exist for as long as there is at least
  one reference to it.

6.12   The NVECTOR_MANYVECTOR implementation

The NVECTOR_MANYVECTOR implementation of the NVECTOR module provided with SUNDIALS is
designed to facilitate problems with an inherent data partitioning for the solution vector. These
data partitions are entirely user-defined, through construction of distinct NVECTOR modules for each
component, that are then combined together to form the NVECTOR_MANYVECTOR. We envision three
generic use cases for this implementation:

A. *Heterogeneous computational architectures (serial or parallel)*: for users who wish to partition
   data on a node between different computing resources, they may create architecture-specific
   subvectors for each partition. For example, a user could create one MPI-parallel component
   based on NVECTOR_PARALLEL, another single-node component for GPU accelerators based on
   NVECTOR_CUDA, and another threaded single-node component based on NVECTOR_OPENMP.

B. *Process-based multiphysics decompositions (parallel)*: for users who wish to combine separate
   simulations together, e.g., where one subvector resides on one subset of MPI processes, while
   another subvector resides on a different subset of MPI processes, and where the user has created
   a MPI *intercommunicator* to connect these distinct process sets together.

C. *Structure of arrays (SOA) data layouts (serial or parallel)*: for users who wish to create separate
   subvectors for each solution component, e.g., in a Navier-Stokes simulation they could have
   separate subvectors for density, velocities and pressure, which are combined together into a
   single NVECTOR_MANYVECTOR for the overall "solution".

We note that the above use cases are not mutually exclusive, and the NVECTOR_MANYVECTOR imple-
mentation should support arbitrary combinations of these cases.

   The NVECTOR_MANYVECTOR implementation is designed to work with any NVECTOR subvectors
that implement the minimum *required* set of operations, however significant performance benefits may
be obtained when subvectors additionally implement the optional local reduction operations listed in
Table 6.5.

   Additionally, NVECTOR_MANYVECTOR sets no limit on the number of subvectors that may be
attached (aside from the limitations of using sunindextype for indexing, and standard per-node
memory limitations). However, while this ostensibly supports subvectors with one entry each (i.e., one

subvector for each solution entry), we anticipate that this extreme situation will hinder performance due to non-stride-one memory accesses and increased function call overhead. We therefore recommend a relatively coarse partitioning of the problem, although actual performance will likely be problem-dependent.

As a final note, in the coming years we plan to introduce additional algebraic solvers and time integration modules that will leverage the problem partitioning enabled by NVECTOR_MANYVECTOR. However, even at present we anticipate that users will be able to leverage such data partitioning in their problem-defining ODE right-hand side, DAE residual, or nonlinear solver residual functions.

6.12.1   NVECTOR_MANYVECTOR structure

The NVECTOR_MANYVECTOR implementation defines the *content* field of N_Vector to be a structure containing the MPI communicator (or SUNMPI_COMM_NULL if running in serial), the number of subvectors comprising the ManyVector, the global length of the ManyVector (including all subvectors on all MPI tasks), a pointer to the beginning of the array of subvectors, and a boolean flag own_data indicating ownership of the subvectors that populate subvec_array.

```
struct _N_VectorContent_ManyVector {
  SUNMPI_Comm    comm;               /* overall MPI communicator      */
  sunindextype   num_subvectors;     /* number of vectors attached    */
  sunindextype   global_length;      /* overall manyvector length     */
  N_Vector*      subvec_array;       /* pointer to N_Vector array      */
  booleantype    own_data;           /* flag indicating data ownership */
};
```

The header file to include when using this module is nvector_manyvector.h. The installed module library to link against is libsundials_nvecmanyvector.*lib* where *.lib* is typically .so for shared libraries and .a for static libraries.

Note: If SUNDIALS is configured with MPI enabled, then the ManyVector library will be built for the parallel use case and SUNMPI_Comm is set to MPI_Comm. As such an MPI-aware compiler will become necessary even in single node uses of the ManyVector library. If SUNDIALS is configured with MPI disabled, then the ManyVector library is built for the single-node (serial) use case and SUNMPI_Comm is set to int. As such, users need not include mpi.h, nor must executables be built with an MPI-aware compiler. For more details see Appendix A.

6.12.2   NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 6.2, 6.3, 6.4, and 6.5, except for N_VGetArrayPointer, N_VSetArrayPointer, N_VScaleAddMultiVectorArray, and N_VLinearCombinationVectorArray. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. Instead, the NVECTOR_MANYVECTOR module provides functions to access subvectors, whose data may in turn be accessed according to their NVECTOR implementations.

The names of vector operations are obtained from those in Tables 6.2, 6.3, 6.4, and 6.5 by appending the suffix _ManyVector (e.g. N_VDestroy_ManyVector). The module NVECTOR_MANYVECTOR provides the following additional user-callable routines:

N_VNew_ManyVector

Prototype   N_Vector N_VNew_ManyVector(sunindextype num_subvectors,
                                           N_Vector *vec_array);

Description   This function creates a ManyVector from a set of existing NVECTOR objects, under the requirement that all MPI-aware subvectors use the same MPI communicator (this is checked internally). If none of the subvectors are MPI-aware, then this may equivalently

be used to describe data partitioning within a single node. We note that this routine is designed to support use cases A and C above.

This routine will copy all `N_Vector` pointers from the input `vec_array`, so the user may modify/free that pointer array after calling this function. However, this routine does *not* allocate any new subvectors, so the underlying NVECTOR objects themselves should not be destroyed before the ManyVector that contains them.

Upon successful completion, the new ManyVector is returned; otherwise this routine returns `NULL` (e.g., if two MPI-aware subvectors use different MPI communicators).

`N_VMake_ManyVector`

Prototype   `N_Vector N_VMake_ManyVector(void *comm, sunindextype num_subvectors,`
                                    `N_Vector *vec_array);`

Description   This function creates a ManyVector from a set of existing NVECTOR objects, and a user-created MPI communicator that "connects" these subvectors. Any MPI-aware subvectors may use different MPI communicators than the input `comm`. We note that this routine is designed to support any combination of the use cases above.

The input `comm` should be the memory reference to this user-created MPI communicator. We note that since many MPI implementations `#define MPI_COMM_WORLD` to be a specific integer *value* (that has no memory reference), users who wish to supply `MPI_COMM_WORLD` to this routine should first duplicate this to a specific `MPI_Comm` variable before passing in the reference, e.g.

```
MPI_Comm comm;
N_Vector x;
MPI_Comm_dup(MPI_COMM_WORLD, &comm);
x = N_VMake_ManyVector(&comm, ...);
```

This routine will internally call `MPI_Comm_dup` to create a copy of the input `comm`, so the user-supplied `comm` argument need not be retained after the call to `N_VMake_ManyVector`.

If all subvectors are MPI-unaware, then the input `comm` argument should be `NULL`, although in this case, it would be simpler to call `N_VNew_ManyVector` instead.

This routine will copy all `N_Vector` pointers from the input `vec_array`, so the user may modify/free that pointer array after calling this function. However, this routine does *not* allocate any new subvectors, so the underlying NVECTOR objects themselves should not be destroyed before the ManyVector that contains them.

Upon successful completion, the new ManyVector is returned; otherwise this routine returns `NULL` (e.g., if the input `vec_array` is `NULL`).

`N_VGetSubvector_ManyVector`

Prototype   `N_Vector N_VGetSubvector_ManyVector(N_Vector v, sunindextype vec_num);`

Description   This function returns the `vec_num` subvector from the NVECTOR array.

`N_VGetNumSubvectors_ManyVector`

Prototype   `sunindextype N_VGetNumSubvectors_ManyVector(N_Vector v);`

Description   This function returns the overall number of subvectors in the ManyVector object.

By default all fused and vector array operations are disabled in the NVECTOR_MANYVECTOR module, except for `N_VWrmsNormVectorArray` and `N_VWrmsNormMaskVectorArray`, that are enabled by default. 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_ManyVector` or `N_VMake_ManyVector`, 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 that the new vectors will have the same operations enabled/disabled, since cloned vectors inherit those configuration options from the vector they are cloned from, while vectors created with N_VNew_ManyVector and N_VMake_ManyVector will have the default settings for the NVECTOR_MANYVECTOR module. We note that these routines *do not* call the corresponding routines on subvectors, so those should be set up as desired *before* attaching them to the ManyVector in N_VNew_ManyVector or N_VMake_ManyVector.

N_VEnableFusedOps_ManyVector

Prototype   int N_VEnableFusedOps_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableLinearCombination_ManyVector

Prototype   int N_VEnableLinearCombination_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableScaleAddMulti_ManyVector

Prototype   int N_VEnableScaleAddMulti_ManyVector(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 ManyVector. The return value is 0 for success and -1 if the input vector or its ops structure are NULL.

N_VEnableDotProdMulti_ManyVector

Prototype   int N_VEnableDotProdMulti_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableLinearSumVectorArray_ManyVector

Prototype   int N_VEnableLinearSumVectorArray_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableScaleVectorArray_ManyVector

Prototype   int N_VEnableScaleVectorArray_ManyVector(N_Vector v, booleantype tf);

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

N_VEnableConstVectorArray_ManyVector

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

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

N_VEnableWrmsNormVectorArray_ManyVector

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

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

N_VEnableWrmsNormMaskVectorArray_ManyVector

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

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

Notes

- `N_VNew_ManyVector` and `N_VMake_ManyVector` set the field *own_data* = `SUNFALSE`.
  `N_VDestroy_ManyVector` will not attempt to call `N_VDestroy` on any subvectors contained in the
  subvector array for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's
  responsibility to deallocate the subvectors.

- To maximize efficiency, arithmetic vector operations in the NVECTOR_MANYVECTOR implemen-
  tation that have more than one `N_Vector` argument do not check for consistent internal repre-
  sentation 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 subvector representations.

6.13   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_VGetLength`: Compares self-reported length to calculated length.

- `Test_N_VGetCommunicator`: Compares self-reported communicator to the one used in constructor; or for MPI-unaware vectors it ensures that NULL is reported.

- `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: $Z[i] = c[0]\,X[0][i] + c[1]\,X[1][i] + c[2]\,X[2][i]$

- `Test_N_VDotProdLocal`: Calculate MPI task-local portion of the dot product of two vectors.

- `Test_N_VMaxNormLocal`: Create vector with known values, find and validate the MPI task-local portion of the max norm.

- `Test_N_VMinLocal`: Create vector, find and validate the MPI task-local min.

- `Test_N_VL1NormLocal`: Create vector, find and validate the MPI task-local portion of the L1 norm.

- `Test_N_VWSqrSumLocal`: Create vector of known values, find and validate the MPI task-local portion of the weighted squared sum of two vectors.

- `Test_N_VWSqrSumMaskLocal`: Create vector of known values, find and validate the MPI task-local portion of the weighted squared sum of two vectors, using all elements except one.

- `Test_N_VInvTestLocal`: Test the MPI task-local portion of z[i] = 1 / x[i]

- `Test_N_VConstrMaskLocal`: Test the MPI task-local portion of the mask of vector x with vector c.

- `Test_N_VMinQuotientLocal`: Fill two vectors with known values. Calculate and validate the MPI task-local minimum quotient.

Chapter 7

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.

7.1   The SUNMatrix API

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          (*matvecsetup)(SUNMatrix)
  int          (*matvec)(SUNMatrix, N_Vector, N_Vector);
  int          (*space)(SUNMatrix, long int*, long int*);
};
```

Table 7.1: 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_SLUNRLOC	Adapter for the SuperLU_DIST `SuperMatrix`	3
SUNMATRIX_CUSTOM	User-provided custom matrix	4

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 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 7.2 contains a complete list of all matrix operations defined by the generic SUNMATRIX module.

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 7.1. It is recommended that a user-supplied SUNMATRIX implementation use the `SUNMATRIX_CUSTOM` identifier.

7.1.1   SUNMatrix functions

The generic `SUNMatrix` object defines the following set of operations:

Table 7.2: 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 7.1.
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.
	continued on next page

Name	Usage and Description
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 of type int and is a SUNMatrix error code 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 of type int and is a SUNMatrix error code 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 of type int and is a SUNMatrix error code denoting success/failure of the operation.
SUNMatScaleAdd	ier = SUNMatScaleAdd(c, A, B); Performs the operation $A = cA + B$. The return value is of type int and is a SUNMatrix error code denoting success/failure of the operation.
SUNMatScaleAddI	ier = SUNMatScaleAddI(c, A); Performs the operation $A = cA + I$. The return value is of type int and is a SUNMatrix error code denoting success/failure of the operation.
SUNMatMatvecSetup	ier = SUNMatMatvecSetup(A); Performs any setup necessary to perform a matrix-vector product. The return value is of type int and is a SUNMatrix error code denoting success/failure of the operation. It is useful for SUNMatrix implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product.
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 of type int and is a SUNMatrix error code denoting success/failure of the operation.

7.1.2 SUNMatrix error codes

The functions provided to SUNMATRIX modules within the SUNDIALS-provided SUNMATRIX implementations utilize a common set of return codes, shown in Table 7.3. These adhere to a common pattern: 0 indicates success, and a negative value indicates a failure. The actual values of each error code are primarily to provide additional information to the user in case of a failure.

Table 7.3: Description of the `SUNMatrix` error codes

Name	Value	Description
SUNMAT_SUCCESS	0	successful call or converged solve
SUNMAT_ILL_INPUT	-1	an illegal input has been provided to the function
SUNMAT_MEM_FAIL	-2	failed memory access or allocation
SUNMAT_OPERATION_FAIL	-3	a SUNMatrix operation returned nonzero
SUNMAT_MATVEC_SETUP_REQUIRED	-4	the `SUNMatMatvecSetup` routine needs to be called before calling `SUNMatMatvec`

7.2   Comaptibility of SUNMatrix modules

We note that not all SUNMATRIX types are compatible with all NVECTOR types provided with SUNDI-ALS. 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 8. More specifically, in Table 7.4 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 7.4: 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	✓		✓	✓					✓
Band	✓		✓	✓					✓
Sparse	✓		✓	✓					✓
SLUNRloc	✓	✓	✓	✓	✓	✓			✓
User supplied	✓	✓	✓	✓	✓	✓	✓	✓	✓

7.3   Implementing a custom SUNMatrix

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`.

7.4   SUNMatrix functions used by IDA

In Table 7.5, we list the matrix functions in the SUNMATRIX module used within the IDA package. The table also shows, for each function, which of the code modules uses the function. The main IDA 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 IDA user does not need to know anything about the usage of matrix functions by the IDA code modules in order to use IDA. The information is presented as an implementation detail for the interested reader.

Table 7.5: List of matrix functions usage by IDA code modules

	IDALS	IDABBDPRE
SUNMatGetID	✓	
SUNMatDestroy		✓
SUNMatZero	✓	✓
SUNMatSpace		†

The matrix functions listed in Table 7.2 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 7.2 that are *not* used by IDA are: `SUNMatCopy`, `SUNMatClone`, `SUNMatScaleAdd`, `SUNMatScaleAddI` and `SUNMatMatvec`. Therefore a user-supplied SUNMATRIX module for IDA could omit these functions.

7.5   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 $0 \leq i < M$ and $0 \leq j < N$) may be accessed via `data[j*M+i]`.

ldata - length of the data array ($= M \cdot N$).

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 $0 \leq i < M$ and $0 \leq j < N$) may be accessed via `cols[j][i]`.

The header file to include when using this module is `sunmatrix/sunmatrix_dense.h`. The SUNMA-TRIX_DENSE module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixdense` module library.

7.5.1   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 $M \times N$ 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 $M \times N$ 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] )
```

7.5.2 SUNMatrix_Dense functions

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix _Dense (e.g. SUNMatCopy_Dense). All the standard matrix operations listed in 7.2 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 $M - 1$.

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.

7.5.3   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.

7.6   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 7.1. 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, $0 \leq mu < N$

ml   - lower half-bandwidth, $0 \leq ml < N$

s_mu   - storage upper bandwidth, $mu \leq s\_mu < N$. 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 ($ldim \geq s\_mu+ml+1$)

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 ($= ldim \cdot N$)

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

Figure 7.1: 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.

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 $\leq i \leq j+$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.

7.6.1 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:

```
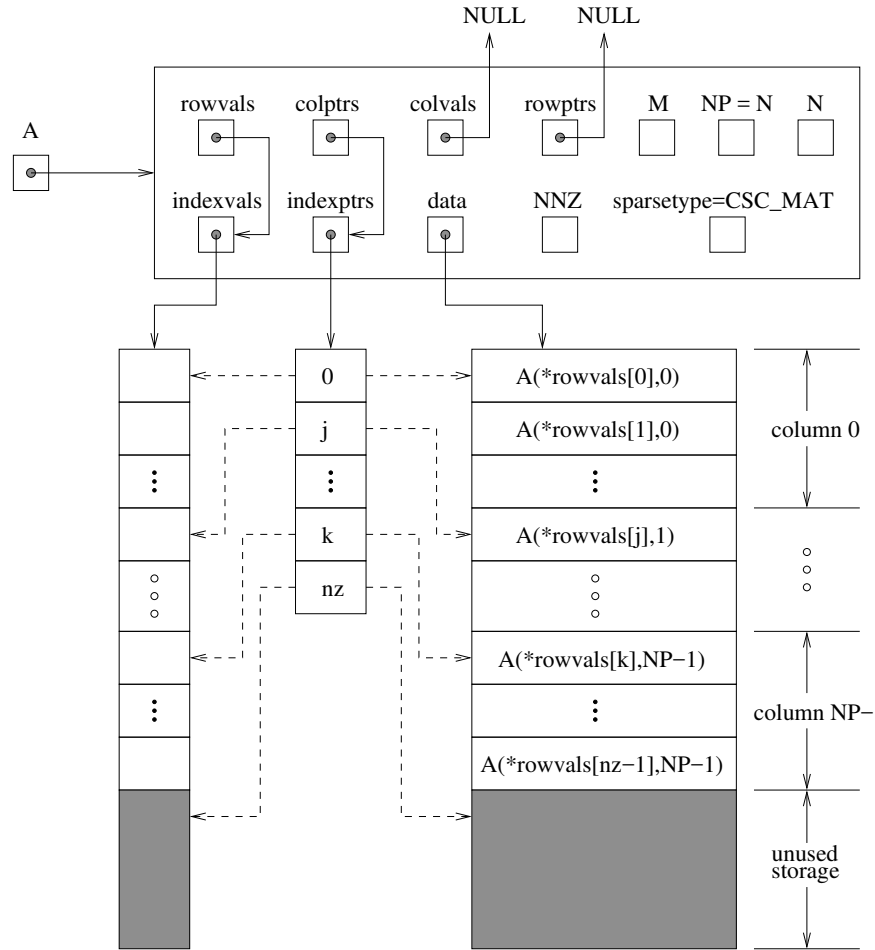#define SM_CONTENT_B(A)       ( (SUNMatrixContent_Band)(A->content) )
```

- 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 $N \times N$ 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 $N \times N$ band matrix A, $0 \le$ j $\le N - 1$. The type of the expression SM_COLUMN_B(A,j) is `realtype *`. The pointer returned by the call SM_COLUMN_B(A,j) can be treated as an array which is indexed from $-$mu to ml.

  The assignments SM_COLUMN_ELEMENT_B(col_j,i,j) = a_ij and
  a_ij = SM_COLUMN_ELEMENT_B(col_j,i,j) reference the (i,j)-th entry of the band matrix A when used in conjunction with SM_COLUMN_B to reference the j-th column through col_j. The index (i,j) should satisfy j$-$mu $\le$ i $\le$ j$+$ml.

  Implementation:

```
#define SM_COLUMN_B(A,j)    ( ((SM_CONTENT_B(A)->cols)[j])+SM_SUBAND_B(A) )
#define SM_COLUMN_ELEMENT_B(col_j,i,j) (col_j[(i)-(j)])
#define SM_ELEMENT_B(A,i,j)
            ( (SM_CONTENT_B(A)->cols)[j][(i)-(j)+SM_SUBAND_B(A)] )
```

7.6.2   SUNMatrix_Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix _Band (e.g. SUNMatCopy_Band). All the standard matrix operations listed in 7.2 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 inter-
               face 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.

7.6.3   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 interoperat-
ing 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 SUNMA-
TRIX_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.

7.7   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 7.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

M   - number of rows

N   - number of columns

NNZ   - maximum number of nonzero entries in the matrix (allocated length of `data` and `indexvals` arrays)

NP   - number of index pointers (e.g. number of column pointers for CSC matrix). For CSC matrices NP = N, and for CSR matrices NP = M. This value is set automatically based the input for `sparsetype`.

data   - pointer to a contiguous block of `realtype` variables (of length NNZ), containing the values of the nonzero entries in the matrix

sparsetype   - type of the sparse matrix (CSC_MAT or CSR_MAT)

indexvals   - pointer to a contiguous block of `int` variables (of length NNZ), containing the row indices (if CSC) or column indices (if CSR) of each nonzero matrix entry held in `data`

indexptrs   - pointer to a contiguous block of `int` variables (of length NP+1). For CSC matrices each entry provides the index of the first column entry into the `data` and `indexvals` arrays, e.g. if `indexptr[3]=7`, then the first nonzero entry in the fourth column of the matrix is located in `data[7]`, and is located in row `indexvals[7]` of the matrix. The last entry contains the total number of nonzero values in the matrix and hence points one past the end of the active data in the `data` and `indexvals` arrays. For CSR matrices, each entry provides the index of the first row entry into the `data` and `indexvals` arrays.

The following pointers are added to the `SlsMat` type for user convenience, to provide a more intuitive interface to the CSC and CSR sparse matrix data structures. They are set automatically when creating a sparse SUNMATRIX, based on the sparse matrix storage type.

rowvals - pointer to `indexvals` when `sparsetype` is CSC_MAT, otherwise set to NULL.

colptrs - pointer to `indexptrs` when `sparsetype` is CSC_MAT, otherwise set to NULL.

colvals - pointer to `indexvals` when `sparsetype` is CSR_MAT, otherwise set to NULL.

rowptrs - pointer to `indexptrs` when `sparsetype` is CSR_MAT, otherwise set to NULL.

For example, the 5×4 CSC matrix

$$\begin{bmatrix} 0 & 3 & 1 & 0 \\ 3 & 0 & 0 & 2 \\ 0 & 7 & 0 & 0 \\ 1 & 0 & 0 & 9 \\ 0 & 0 & 0 & 5 \end{bmatrix}$$

could be stored in this structure as either

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4};
indexptrs = {0, 2, 4, 5, 8};
```

or

```
M = 5;
N = 4;
NNZ = 10;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0, *, *};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4, *, *};
indexptrs = {0, 2, 4, 5, 8};
```

where the first has no unused space, and the second has additional storage (the entries marked with
* may contain any values). Note in both cases that the final value in `indexptrs` is 8, indicating the
total number of nonzero entries in the matrix.

Similarly, in CSR format, the same matrix could be stored as

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 2.0, 7.0, 1.0, 9.0, 5.0};
sparsetype = CSR_MAT;
indexvals = {1, 2, 0, 3, 1, 0, 3, 3};
indexptrs = {0, 2, 4, 5, 7, 8};
```

The header file to include when using this module is `sunmatrix/sunmatrix_sparse.h`. The SUNMA-
TRIX_SPARSE module is accessible from all SUNDIALS solvers *without* linking to the
`libsundials_sunmatrixsparse` module library.

7.7.1   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.

Figure 7.2: Diagram of the storage for a compressed-sparse-column matrix. Here A is an M × 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 M − 1, corresponding to the row index (zero-based) of each nonzero value. The entries in data contain the values of the nonzero entries, with the row i, column j entry of A (again, zero-based) denoted as A(i,j). The indexptrs array contains N + 1 entries; the first N denote the starting index of each column within the indexvals and data arrays, while the final entry points one past the final nonzero entry. Here, although NNZ values are allocated, only nz are actually filled in; the greyed-out portions of data and indexvals indicate extra allocated space.

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 )
```

7.7.2   SUNMatrix_Sparse functions

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). All the standard matrix operations listed in 7.2 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.

7.7.3   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.

7.8 The SUNMatrix_SLUNRloc implementation

The SUNMATRIX_SLUNRLOC implementation of the SUNMATRIX module provided with SUNDIALS is an adapter for the `SuperMatrix` structure provided by the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li [2, 22, 32, 33]. It is designed to be used with the SUNLIN-SOL_SUPERLUDIST linear solver discussed in Section 8.10. To this end, it defines the *content* field of `SUNMatrix` to be the following structure:

```
struct _SUNMatrixContent_SLUNRloc {
  booleantype    own_data;
  gridinfo_t     *grid;
  sunindextype   *row_to_proc;
  pdgsmv_comm_t  *gsmv_comm;
  SuperMatrix    *A_super;
  SuperMatrix    *ACS_super;
};
```

A more complete description of the this *content* field is given below:

own_data - a flag which indicates if the SUNMatrix is responsible for freeing `A_super`

grid - pointer to the SuperLU_DIST structure that stores the 2D process grid

row_to_proc - a mapping between the rows in the matrix and the process it resides on; will be `NULL` until the `SUNMatMatvecSetup` routine is called

gsmv_comm - pointer to the SuperLU_DIST structure that stores the communication information needed for matrix-vector multiplication; will be `NULL` until the `SUNMatMatvecSetup` routine is called

A_super - pointer to the underlying SuperLU_DIST `SuperMatrix` with `Stype = SLU_NR_loc, Dtype = SLU_D, Mtype = SLU_GE`; must have the full diagonal present to be used with `SUNMatScaleAddI` routine

ACS_super - a column-sorted version of the matrix needed to perform matrix-vector multiplication; will be `NULL` until the routine `SUNMatMatvecSetup` routine is called

The header file to include when using this module is `sunmatrix/sunmatrix_slunrloc.h`. The installed module library to link to is `libsundials_sunmatrixslunrloc.`*lib* where *.lib* is typically `.so` for shared libraries and `.a` for static libraries.

7.8.1 SUNMatrix_SLUNRloc functions

The module SUNMATRIX_SLUNRLOC provides the following user-callable routines:

SUNMatrix_SLUNRloc

Call	`A = SUNMatrix_SLUNRloc(Asuper, grid);`
Description	The function `SUNMatrix_SLUNRloc` creates and allocates memory for a SUNMATRIX_SLUNRLOC object.
Arguments	`Asuper` (`SuperMatrix*`) a fully-allocated SuperLU_DIST `SuperMatrix` that the SUN-Matrix will wrap; must have `Stype = SLU_NR_loc, Dtype = SLU_D, Mtype = SLU_GE` to be compatible
	`grid` (`gridinfo_t*`) the initialized SuperLU_DIST 2D process grid structure
Return value	a `SUNMatrix` object if `Asuper` is compatible else `NULL`
Notes	

| SUNMatrix_SLUNRloc_Print |

Call   SUNMatrix_SLUNRloc_Print(A, fp);

Description   The function SUNMatrix_SLUNRloc_Print prints the underlying SuperMatrix content.

Arguments   A   (SUNMatrix) the matrix to print
              fp (FILE) the file pointer used for printing

Return value void

Notes

| SUNMatrix_SLUNRloc_SuperMatrix |

Call   Asuper = SUNMatrix_SLUNRloc_SuperMatrix(A);

Description   The function SUNMatrix_SLUNRloc_SuperMatrix provides access to the underlying Su-
              perLU_DIST SuperMatrix of A.

Arguments   A   (SUNMatrix) the matrix to access

Return value SuperMatrix*

Notes

| SUNMatrix_SLUNRloc_ProcessGrid |

Call   grid = SUNMatrix_SLUNRloc_ProcessGrid(A);

Description   The function SUNMatrix_SLUNRloc_ProcessGrid provides access to the SuperLU_DIST
              gridinfo_t structure associated with A.

Arguments   A   (SUNMatrix) the matrix to access

Return value gridinfo_t*

Notes

| SUNMatrix_SLUNRloc_OwnData |

Call   does_own_data = SUNMatrix_SLUNRloc_OwnData(A);

Description   The function SUNMatrix_SLUNRloc_OwnData returns true if the SUNMatrix object is
              responsible for freeing A_super, otherwise it returns false.

Arguments   A   (SUNMatrix) the matrix to access

Return value booleantype

Notes

The SUNMATRIX_SLUNRLOC module defines implementations of all generic SUNMatrix operations
listed in Table 7.2:

- SUNMatGetID_SLUNRloc - returns SUNMATRIX_SLUNRLOC

- SUNMatClone_SLUNRloc

- SUNMatDestroy_SLUNRloc

- SUNMatSpace_SLUNRloc - this only returns information for the storage within the matrix inter-
  face, i.e. storage for row_to_proc

- SUNMatZero_SLUNRloc

- SUNMatCopy_SLUNRloc

- `SUNMatScaleAdd_SLUNRloc` - performs $A = cA + B$, but A and B must have the same sparsity pattern

- `SUNMatScaleAddI_SLUNRloc` - performs $A = cA + I$, but the diagonal of A must be present

- `SUNMatMatvecSetup_SLUNRloc` - initializes the SuperLU_DIST parallel communication structures needed to perform a matrix-vector product; only needs to be called before the first call to `SUNMatMatvec` or if the matrix changed since the last setup

- `SUNMatMatvec_SLUNRloc`

The SUNMATRIX_SLUNRLOC module requires that the complete diagonal, i.e. nonzeros and zeros, is present in order to use the `SUNMatScaleAddI` operation.

Chapter 8

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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{8.1}$$

where

$$
\begin{aligned}
\tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\
\tilde{b} &= S_1 P_1^{-1} b, \\
\tilde{x} &= S_2 P_2 x,
\end{aligned}
\tag{8.2}
$$

and where

- P_1 is the left preconditioner,

- P_2 is the right preconditioner,

- S_1 is a diagonal matrix of scale factors for $P_1^{-1}b$,

- S_2 is a diagonal matrix of scale factors for $P_2 x$.

The scaling matrices are chosen so that $S_1 P_1^{-1} b$ and $S_2 P_2 x$ have dimensionless components. If preconditioning is done on the left only ($P_2 = I$), by a matrix P, then S_2 must be a scaling for x, while S_1 is a scaling for $P^{-1}b$, and so may also be taken as a scaling for x. Similarly, if preconditioning is done on the right only ($P_1 = I$ and $P_2 = P$), then S_1 must be a scaling for b, while S_2 is a scaling for Px, and may also be taken as a scaling for b.

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 §8.4.2 for more details). In this case, they instead request that iterative linear solvers stop based on the criteria

$$\left\| P_1^{-1} b - P_1^{-1} A x \right\|_2 < \text{tol}.$$

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 8.1.1 – 8.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 8.1.4. A table of linear solver return codes is given in section 8.1.5. The `SUNLinearSolver` type and the generic SUNLINSOL module are defined in section 8.1.6. The section 8.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 8.3 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 8.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

8.1 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`.

8.1.1 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 8.3.1 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 8.1.

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 8.1.

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 8.1.

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.

8.1.2   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 8.1.

| 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 (8.1)-(8.2). 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 8.1.

| 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 (8.1)-(8.2), 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 8.1.

8.1.3   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 8.1.

Notes   This function is advisory only, for use in determining a user's total space requirements.

8.1.4   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 alloced 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 alloced 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

$$\|Pz - r\|_{\mathrm{wrms}} < tol$$

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.

8.1.5   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 8.1. 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 8.1: 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)

8.1.6   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 8.1.1-8.1.3. 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));
}
```

8.2   Compatibility of `SUNLinearSolver` modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 8.2 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 8.2: SUNDIALS matrix-based linear solvers and matrix implementations that can be used for each.

Linear Solver Interface	Dense Matrix	Banded Matrix	Sparse Matrix	SLUNRloc Matrix	User Supplied
Dense	✓				✓
Band		✓			✓
LapackDense	✓				✓
LapackBand		✓			✓
KLU			✓		✓
SuperLU_DIST				✓	✓
SUPERLUMT			✓		✓
continued on next page					

Linear Solver Interface	Dense Matrix	Banded Matrix	Sparse Matrix	SLUNRloc Matrix	User Supplied
User supplied	✓	✓	✓	✓	✓

8.3   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 8.4 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.

8.3.1   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 7.4 and 8.4 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 7 and 8. *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 8.4.2 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 8. *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.

8.4 IDA SUNLinearSolver interface

Table 8.3 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 8.3: 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.

8.4.1   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

$$x = \frac{2}{1 + \alpha/\bar{\alpha}}\bar{x}. \tag{8.3}$$

For values of $\alpha/\bar{\alpha}$ that are "close" to 1, this rescaling approximately solves the original linear system.

8.4.2   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 (8.1)-(8.2)):

$$\left\| \tilde{b} - \tilde{A}\tilde{x} \right\|_2 < \text{tol}$$
$$\Leftrightarrow \quad \left\| SP_1^{-1}b - SP_1^{-1}Ax \right\|_2 < \text{tol}$$
$$\Leftrightarrow \quad \sum_{i=0}^{n-1} \left[W_i \left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2$$
$$\Leftrightarrow \quad W_{mean}^2 \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2$$
$$\Leftrightarrow \quad \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \left(\frac{\text{tol}}{W_{mean}} \right)^2$$
$$\Leftrightarrow \quad \left\| P_1^{-1}(b - Ax) \right\|_2 < \frac{\text{tol}}{W_{mean}}$$

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.

8.5   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.

8.5.1   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).

8.5.2   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 8.1.1 – 8.1.3:

- `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.

8.5.3   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.

8.5.4 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.

8.6   The SUNLinearSolver_Band implementation

This section describes the SUNLINSOL implementation for solving banded linear systems. The SUNLIN-SOL_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.

8.6.1   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`.

8.6.2   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 8.1.1 – 8.1.3:

- `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.

8.6.3   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.

8.6.4   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.

8.7   The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LA-
PACK. The SUNLINSOL_LAPACKDENSE module is designed to be used with the corresponding SUNMA-
TRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVEC-
TOR_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`.

8.7.1 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).

8.7.2 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 8.1.1 – 8.1.3:

- `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

8.7.3   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.

8.7.4   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.

8.8   The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LA-PACK. 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.

8.8.1   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.

8.8.2   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 8.1.1 – 8.1.3:

- 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

8.8.3   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.

8.8.4 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.

8.9 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, 16]. 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.

8.9.1 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.

8.9.2 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 8.1.1 – 8.1.3:

- 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 identical 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 identical input and output arguments is also provided.

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

8.9.3   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 SUN-LINSOL_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.

8.9.4 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).

8.10   The SUNLinearSolver_SuperLUDIST implementation

The SuperLU_DIST implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL_SUPERLUDIST, is designed to be used with the corresponding SUNMATRIX_SLUNRLOC matrix type, and one of the serial, threaded or parallel NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, NVECTOR_PTHREADS, NVECTOR_PARALLEL, or NVECTOR_PARHYP).

The header file to include when using this module is `sunlinsol/sunlinsol_superludist.h`. The installed module library to link to is `libsundials_sunlinsolsuperludist.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

8.10.1   SUNLinearSolver_SuperLUDIST description

The SUNLINSOL_SUPERLUDIST module is a SUNLINSOL adapter for the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li [2, 22, 32, 33]. The package uses a SPMD parallel programming model and multithreading to enhance efficiency in distributed-memory parallel environments with multicore nodes and possibly GPU accelerators. It uses MPI for communication, OpenMP for threading, and CUDA for GPU support. In order to use the SUNLINSOL_SUPERLUDIST interface to SuperLU_DIST, it is assumed that SuperLU_DIST has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SuperLU_DIST (see Appendix A for details). Additionally, the adapter only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to use single or extended precision. Moreover, since the SuperLU_DIST library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SuperLU_DIST library is installed using the same integer size as SUNDIALS.

The SuperLU_DIST library provides many options to control how a linear system will be solved. These options may be set by a user on an instance of the `superlu_dist_options_t` struct, and then it may be provided as an argument to the SUNLINSOL_SUPERLUDIST constructor. The SUNLINSOL_SUPERLUDIST module will respect all options set except for `Fact` – this option is necessarily modified by the SUNLINSOL_SUPERLUDIST module in the setup and solve routines.

Since the linear systems that arise within the context of SUNDIALS calculations will typically have identical sparsity patterns, the SUNLINSOL_SUPERLUDIST module is constructed to perform the following operations:

- The first time that the "setup" routine is called, it sets the SuperLU_DIST option `Fact` to `DOFACT` so that a subsequent call to the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to solve the system.

- On subsequent calls to the "setup" routine, it sets the SuperLU_DIST option `Fact` to `SamePattern` so that a subsequent call to "solve" will perform factorization assuming the same sparsity pattern as prior, i.e. it will reuse the column permutation vector.

- If "setup" is called prior to the "solve" routine, then the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to the sparse triangular solves, and, potentially, iterative refinement. If "setup" is not called prior, "solve" will skip to the triangular solve step. We note that in this solve SuperLU_DIST operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.10.2   SUNLinearSolver_SuperLUDIST functions

The SUNLINSOL_SUPERLUDIST module defines implementations of all "direct" linear solver operations listed in Sections 8.1.1-8.1.3:

- `SUNLinSolGetType_SuperLUDIST`

- `SUNLinSolInitialize_SuperLUDIST` – this sets the `first_factorize` flag to 1 and resets the internal SuperLU_DIST statistics variables.

- `SUNLinSolSetup_SuperLUDIST` – this sets the appropriate SuperLU_DIST options so that a subsequent solve will perform a symbolic and numerical factorization before proceeding with the triangular solves

- `SUNLinSolSolve_SuperLUDIST` – this calls the SuperLU_DIST solve routine to perform factorization (if the setup routine was called prior) and then use the *LU* factors to solve the linear system.

- `SUNLinSolLastFlag_SuperLUDIST`

- `SUNLinSolSpace_SuperLUDIST` – 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 SuperLU_DIST documentation.

- `SUNLinSolFree_SuperLUDIST`

In addition, the module SUNLINSOL_SUPERLUDIST provides the following user-callable routines:

SUNLinSol_SuperLUDIST

Call	`LS = SUNLinSol_SuperLUDIST(y, A, grid, lu, scaleperm, solve, stat, options);`
Description	The function `SUNLinSol_SuperLUDIST` creates and allocates memory for a SUNLIN-SOL_SUPERLUDIST object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver
	`A` (`SUNMatrix`) a SUNMATRIX_SLUNRLOC matrix template for cloning matrices needed within the solver
	`grid` (`gridinfo_t*`)
	`lu` (`LUstruct_t*`)
	`scaleperm` (`ScalePermstruct_t*`)
	`solve` (`SOLVEstruct_t*`)
	`stat` (`SuperLUStat_t*`)
	`options` (`superlu_dist_options_t*`)
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 SuperLU_DIST 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_SLUNRLOC matrix type and the NVECTOR_SERIAL, NVECTOR_PARALLEL, NVECTOR_PARHYP, 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 `grid`, `lu`, `scaleperm`, `solve`, and `options` arguments are not checked and are passed directly to SuperLU_DIST routines.
	Some struct members of the `options` argument are modified internally by the SUNLIN-SOL_SUPERLUDIST solver. Specifically the member `Fact`, is modified in the setup and solve routines.

SUNLinSol_SuperLUDIST_GetBerr

Call	`realtype berr = SUNLinSol_SuperLUDIST_GetBerr(LS);`
Description	The function `SUNLinSol_SuperLUDIST_GetBerr` returns the componentwise relative backward error of the computed solution.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value `realtype`

Notes

| SUNLinSol_SuperLUDIST_GetGridinfo |

Call   `gridinfo_t *grid = SUNLinSol_SuperLUDIST_GetGridinfo(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetGridinfo` returns the SuperLU_DIST struc-
             ture that contains the 2D process grid.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value `gridinfo_t*`

Notes

| SUNLinSol_SuperLUDIST_GetLUstruct |

Call   `LUstruct_t *lu = SUNLinSol_SuperLUDIST_GetLUstruct(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetLUstruct` returns the SuperLU_DIST struc-
             ture that contains the distributed L and U factors.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value `LUstruct_t*`

Notes

| SUNLinSol_SuperLUDIST_GetSuperLUOptions |

Call   `superlu_dist_options_t *opts = SUNLinSol_SuperLUDIST_GetSuperLUOptions(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetSuperLUOptions` returns the SuperLU_DIST
             structure that contains the options which control how the linear system is factorized
             and solved.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value `superlu_dist_options_t*`

Notes

| SUNLinSol_SuperLUDIST_GetScalePermstruct |

Call   `ScalePermstruct_t *sp = SUNLinSol_SuperLUDIST_GetScalePermstruct(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetScalePermstruct` returns the SuperLU_DIST
             structure that contains the vectors that describe the transformations done to the matrix,
             A.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value `ScalePermstruct_t*`

Notes

SUNLinSol_SuperLUDIST_GetSOLVEstruct

Call   SOLVEstruct_t *solve = SUNLinSol_SuperLUDIST_GetSOLVEstruct(LS);

Description   The function SUNLinSol_SuperLUDIST_GetSOLVEstruct returns the SuperLU_DIST struc-
                ture that contains information for communication during the solution phase.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   SOLVEstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSuperLUStat

Call   SuperLUStat_t *stat = SUNLinSol_SuperLUDIST_GetSuperLUStat(LS);

Description   The function SUNLinSol_SuperLUDIST_GetSuperLUStat returns the SuperLU_DIST struc-
                ture that stores information about runtime and flop count.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   SuperLUStat_t*

Notes

8.10.3 SUNLinearSolver_SuperLUDIST content

The SUNLINSOL_SUPERLUDIST module defines the *content* field of a SUNLinearSolver to be the fol-
lowing structure:

```
struct _SUNLinearSolverContent_SuperLUDIST {
  booleantype            first_factorize;
  long int               last_flag;
  realtype               berr;
  gridinfo_t             *grid;
  LUstruct_t             *lu;
  superlu_dist_options_t *options;
  ScalePermstruct_t      *scaleperm;
  SOLVEstruct_t          *solve;
  SuperLUStat_t          *stat;
  sunindextype           N;
};
```

These entries of the *content* field contain the following information:

first_factorize - flag indicating whether the factorization has ever been performed,

last_flag - last error return flag from calls to internal routines,

berr - the componentwise relative backward error of the computed solution,

grid - pointer to the SuperLU_DIST structure that stores the 2D process grid,

lu - pointer to the SuperLU_DIST structure that stores the distributed L and U factors,

options - pointer to SuperLU_DIST options structure,

scaleperm - pointer to the SuperLU_DIST structure that stores vectors describing the transforma-
tions done to the matrix, A,

solve - pointer to the SuperLU_DIST solve structure,

stat - pointer to the SuperLU_DIST structure that stores information about runtime and flop count,

N - the number of equations in the system

8.11   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 [3, 31, 18]. 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.

8.11.1   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.

8.11.2   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 8.1.1 – 8.1.3:

- 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.

8.11.3 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 SUN-LINSOL_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.

| FSUNMASSSUPERLUMTSETORDERING |

Call   `FSUNMASSSUPERLUMTSETORDERING(ordering, ier)`

Description The function `FSUNMASSSUPERLUMTSETORDERING` 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.

8.11.4   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.

8.12   The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [37]) 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.

8.12.1   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.

8.12.2   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 8.1.1 – 8.1.3:

- 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.

8.12.3 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 rou-
              tine.

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 rou-
              tine.

8.12.4   SUNLinearSolver_SPGMR content

The SUNLINSOL_SPGMR module defines the *content* field of a SUNLinearSolver as the following struc-
ture:

```
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.

8.13   The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [36]) 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.

8.13.1   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.

8.13.2   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 8.1.1 – 8.1.3:

- 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.

8.13.3   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 SUN-LINSOL_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 rou-
                 tine.

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 rou-
                 tine.

8.13.4 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 $v_1, \ldots, v_{\text{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

Z   - the array of preconditioned Krylov basis vectors $z_1, \ldots, z_{\text{maxl}+1}$, stored in `Z[0]`, ..., `Z[maxl]`. Each z_i is a vector of type NVECTOR.,

Hes   - the $(\text{maxl} + 1) \times \text{maxl}$ 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.

8.14   The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [38]) 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.

8.14.1   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.

8.14.2   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 consis-
                tent 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 precondi-
                tioning (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 precondi-
                tioning 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 in-
                terface module.

The SUNLINSOL_SPBCGS module defines implementations of all "iterative" linear solver operations
listed in Sections 8.1.1 – 8.1.3:

- 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.

8.14.3   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 SUNLIN-SOL_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 SUN-LINSOL_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.

8.14.4   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.

8.15   The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [21]) 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.

8.15.1   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.

8.15.2 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 identical 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 8.1.1 – 8.1.3:

- 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

8.15.3 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.

8.15.4   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.

8.16 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementaiton of the PCG (Preconditioned Conjugate Gradient [23]) 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.

8.16.1 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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{8.4}$$

where

$$
\begin{aligned}
\tilde{A} &= SP^{-1}AP^{-1}S, \\
\tilde{b} &= SP^{-1}b, \\
\tilde{x} &= S^{-1}Px.
\end{aligned}
\tag{8.5}
$$

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:

$$\|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|SP^{-1}b - SP^{-1}Ax\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|P^{-1}b - P^{-1}Ax\|_S < \delta$$

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.

8.16.2   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 8.1.1 – 8.1.3:

- `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.

8.16.3   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 maxi-
            mum 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.

8.16.4   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.

8.17   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 9

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 9.1 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 9.1.1 – 9.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 9.1.4. A table of nonlinear solver return codes is given in section 9.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 9.1.6. Section 9.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 9.1.8 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.

9.1 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`.

9.1.1 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 initial-
               ization 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 non-
               linear 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`.

9.1.2 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 9.1.4 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 9.1.4 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 9.1.4 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 implementa-
               tions 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 conver-
                       gence test function. See section 9.1.4 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 non-
               linear 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).

9.1.3   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 nonlin-
            ear 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 non-
            linear solve. This function is *required* when using SUNDIALS integrator-provided conver-
            gence 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 non-
            linear 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.

9.1.4   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 oc-
              curred 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 mod-
              ules utilizing their own convergence criteria may ignore these functions.

9.1.5   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 9.1. Here, negative values correspond to non-recoverable failures, positive values to
recoverable failures, and zero to a successful call.

Table 9.1: 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

9.1.6   The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic SUN-
NONLINSOL 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 non-
linear 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 9.1.1 – 9.1.3. 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));
}
```

9.1.7 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 6.2 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

9.1.8   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 9.1.1 – 9.1.3.
   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.

9.2   The SUNNonlinearSolver_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton's method. To access the SUNNON-
LINSOL_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.

9.2.1   SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{9.1}$$

given an initial guess $y^{(0)}$, Newton's method computes a series of approximate solutions

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{9.2}$$

where m is the Newton iteration index, and the Newton update $\delta^{(m+1)}$ is the solution of the linear
system

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)}) \,, \tag{9.3}$$

in which A is the Jacobian matrix

$$A \equiv \partial F/\partial y \,. \tag{9.4}$$

Depending on the linear solver used, the SUNNONLINSOL_NEWTON module will employ either a Modi-
fied Newton method, or an Inexact Newton method [6, 10, 17, 19, 30]. 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 infre-
quently 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, SUN-
NONLINSOL_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.

9.2.2 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 9.1.1 – 9.1.3 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 9.1.1 – 9.1.3 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.

9.2.3   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.

9.2.4   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.

9.3   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.

9.3.1   SUNNonlinearSolver_FixedPoint description

To find the solution to

$$G(y) = y \tag{9.5}$$

given an initial guess $y^{(0)}$, the fixed point iteration computes a series of approximate solutions

$$y^{(n+1)} = G(y^{(n)}) \tag{9.6}$$

where n is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [4, 39, 20, 34]. With Anderson acceleration using subspace size m, the series of approximate solutions can be formulated as the linear combination

$$y^{(n+1)} = \sum_{i=0}^{m_n} \alpha_i^{(n)} G(y^{(n-m_n+i)}) \tag{9.7}$$

where $m_n = \min\{m, n\}$ and the factors

$$\alpha^{(n)} = (\alpha_0^{(n)}, \ldots, \alpha_{m_n}^{(n)}) \tag{9.8}$$

solve the minimization problem $\min_\alpha \|F_n \alpha^T\|_2$ under the constraint that $\sum_{i=0}^{m_n} \alpha_i = 1$ where

$$F_n = (f_{n-m_n}, \ldots, f_n) \tag{9.9}$$

with $f_i = G(y^{(i)}) - y^{(i)}$. Due to this constraint, in the limit of $m = 0$ the accelerated fixed point iteration formula (9.7) simplifies to the standard fixed point iteration (9.6).

Following the recommendations made in [39], the SUNNONLINSOL_FIXEDPOINT implementation computes the series of approximate solutions as

$$y^{(n+1)} = G(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} \tag{9.10}$$

with $\Delta g_i = G(y^{(i+1)}) - G(y^{(i)})$ and where the factors

$$\gamma^{(n)} = (\gamma_0^{(n)}, \ldots, \gamma_{m_n-1}^{(n)}) \tag{9.11}$$

solve the unconstrained minimization problem $\min_\gamma \|f_n - \Delta F_n \gamma^T\|_2$ where

$$\Delta F_n = (\Delta f_{n-m_n}, \ldots, \Delta f_{n-1}), \tag{9.12}$$

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.

9.3.2   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 (9.6) does not require the setup or solution of any linear systems, the SUNNONLINSOL_FIXEDPOINT module implements all of the functions defined in sections 9.1.1 – 9.1.3 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 9.1.1 – 9.1.3 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.

9.3.3   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.

9.3.4   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 SUN-DIALS on this system. Back at the command prompt, you can now run:

```
                                        Terminal                          _  □  ×
 File   Edit   View   Search   Terminal   Help
                                      Page 1 of 1
 BLAS_ENABLE                      OFF
 BUILD_ARKODE                     ON
 BUILD_CVODE                      ON
 BUILD_CVODES                     ON
 BUILD_IDA                        ON
 BUILD_IDAS                       ON
 BUILD_KINSOL                     ON
 BUILD_SHARED_LIBS                ON
 BUILD_STATIC_LIBS                ON
 BUILD_TESTING                    ON
 CMAKE_BUILD_TYPE
 CMAKE_C_COMPILER                 /usr/bin/cc
 CMAKE_C_FLAGS
 CMAKE_INSTALL_LIBDIR             lib64
 CMAKE_INSTALL_PREFIX             /usr/casc/sundials/instdir
 CUDA_ENABLE                      OFF
 EXAMPLES_ENABLE_C                ON
 EXAMPLES_ENABLE_CXX              OFF
 EXAMPLES_INSTALL                 ON
 EXAMPLES_INSTALL_PATH            /usr/casc/sundials/instdir/examples
 F2003_INTERFACE_ENABLE           OFF
 F77_INTERFACE_ENABLE             OFF
 HYPRE_ENABLE                     OFF
 KLU_ENABLE                       OFF
 LAPACK_ENABLE                    OFF
 MPI_ENABLE                       OFF
 OPENMP_DEVICE_ENABLE             OFF
 OPENMP_ENABLE                    OFF
 PETSC_ENABLE                     OFF
 PTHREAD_ENABLE                   OFF
 RAJA_ENABLE                      OFF
 SUNDIALS_INDEX_SIZE              64
 SUNDIALS_PRECISION               double
 SUPERLUMT_ENABLE                 OFF
 USE_GENERIC_MATH                 ON
 USE_XSDK_DEFAULTS                OFF


 CMAKE_INSTALL_PREFIX: Install path prefix, prepended onto install directories.
 Press [enter] to edit option                                   CMake Version 3.1.3
 Press [c] to configure        Press [g] to generate and exit
 Press [h] for help            Press [q] to quit without generating
 Press [t] to toggle advanced mode (Currently Off)
```

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

```
% make
```

To install SUNDIALS in the installation directory specified in the configuration, simply run:

```
% make install
```

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 unless Trilinos_ENABLE is ON.

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 informa-
> tion 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. This will build the parallel NVECTOR and the MPI-aware version
> of the ManyVector library.
> 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

SUPERLUDIST_ENABLE - Enable SuperLU_DIST support
Default: OFF
Note: See additional information on building with SuperLU_DIST enabled in A.1.4.

SUPERLUDIST_INCLUDE_DIR - Path to SuperLU_DIST header files (typically SRC directory)

SUPERLUDIST_LIBRARY_DIR - Path to SuperLU_DIST installed library files

SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST

SUPERLUDIST_OpenMP - Enable SUNDIALS support for SuperLU_DIST built with OpenMP
Default: OFF
Note: SuperLU_DIST must be built with OpenMP support for this option to function properly. Additionally the environment variable OMP_NUM_THREADS must be set to the desired number of threads.

SUPERLUMT_ENABLE - Enable SUPERLUMT support
Default: OFF
Note: See additional information on building with SUPERLUMT 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

Trilinos_ENABLE - Enable Trilinos support (build the Tpetra NVECTOR).
Default: OFF

Trilinos_DIR - Path to the Trilinos install directory.
Default:

TRILINOS_INTERFACE_C_COMPILER - **advanced option** - Set the C compiler for building the Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).
Default: The C compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_COMPILER or MPI_C_COMPILER if USE_XSDK_DEFAULTS=ON.
Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_C_COMPILER_FLAGS - **advanced option** - Set the C compiler flags for Trilinos
>   interface (i.e., NVECTOR_TRILINOS and the examples that use it).
>   Default: The C compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF.
>   CMAKE_C_FLAGS if USE_XSDK_DEFAULTS=ON.
>   Note: It is recommended to use the same flags that were used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER - **advanced option** - Set the C++ compiler for builing Trilinos
>   interface (i.e., NVECTOR_TRILINOS and the examples that use it).
>   Default: The C++ compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF.
>   CMAKE_CXX_COMPILER or MPI_CXX_COMPILER if USE_XSDK_DEFAULTS=ON.
>   Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER_FLAGS - **advanced option** - Set the C++ compiler flags for Trili-
>   nos interface (i.e., NVECTOR_TRILINOS and the examples that use it).
>   Default: The C++ compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF.
>   CMAKE_CXX_FLAGS if USE_XSDK_DEFAULTS=ON.
>   Note: Is is recommended to use the same flags that were used to build the Trilinos library.

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_SUPERLUDIST` - Enable SuperLU_DIST support
> Default: OFF
> SUNDIALS equivalent: `SUPERLUDIST_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_SUPERLUDIST_INCLUDE_DIRS` - Path to SuperLU_DIST header files
> SUNDIALS equivalent: `SUPERLUDIST_INCLUDE_DIR`

`TPL_SUPERLUDIST_LIBRARIES` - Semi-colon separated list of libraries needed for SuperLU_DIST including the SuperLU_DIST library itself
> SUNDIALS equivalent: `SUPERLUDIST_LIBRARIES`

`TPL_SUPERLUDIST_OPENMP` - Enable SUNDIALS support for SuperLU_DIST built with OpenMP
> SUNDIALS equivalent: `SUPERLUDIST_OPENMP`

`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 5.3.0. 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 SuperLU_DIST

The SuperLU_DIST libraries are available for download from the Lawrence Berkeley National Laboratory website: `http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_dist`. SUNDIALS has been tested with SuperLU_DIST greater than 6.1. To enable SuperLU_DIST, set `SUPERLUDIST_ENABLE` to `ON`, set `SUPERLUDIST_INCLUDE_DIR` to the include directory of the SuperLU_DIST installation (typically `SRC`), and set the variable `SUPERLUDIST_LIBRARY_DIR` to the path to library directory of the SuperLU_DIST installation (typically `lib`). At the same time, the variable `SUPERLUDIST_LIBRARIES` must be set to a semi-colon separated list of other libraries SuperLU_DIST depends on. For example, if SuperLU_DIST was built with LAPACK, then include the LAPACK library in this list. If SuperLU_DIST was built with OpenMP support, then you may set `SUPERLUDIST_OPENMP` to `ON` to utilize the OpenMP functionality of SuperLU_DIST.

⚠️ Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having `PTHREAD_ENABLE` set to `ON` then SuperLU_DIST should not be set to use OpenMP.

Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: `http://www.mcs.anl.gov/` SUNDIALS has been tested with PETSc version 3.10.3. 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 2.14.0. 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 9.0 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 0.6. 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_CUDA` to `ON`.

Building with Trilinos

Trilinos is a suite of numerical libraries developed by Sandia National Laboratories. It can be obtained at `https://github.com/trilinos/Trilinos`. SUNDIALS Trilinos modules and examples have been tested with Trilinos version 12.14. To enable Trilinos, set `Trilinos_ENABLE` to `ON`. If Trilinos is installed in a nonstandard location you will be prompted to set the variable `Trilinos_DIR` with the path to the Trilinos CMake configuration file. It is desireable to build the Trilinos vector interface with same compiler and options that were used to build Trilinos. CMake will try to find the correct compiler settings automatically from the Trilinos configuration file. If that is not successful, the compilers and options can be manually set with the following CMake variables:

- `Trilinos_INTERFACE_C_COMPILER`

- `Trilinos_INTERFACE_C_COMPILER_FLAGS`

- `Trilinos_INTERFACE_CXX_COMPILER`

- `Trilinos_INTERFACE_CXX_COMPILER_FLAGS`

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
		continued on next page

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NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.*lib*
	Header files	nvector/nvector_petsc.h
NVECTOR_CUDA	Libraries	libsundials_nveccuda.*lib*
	Libraries	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	libsundials_nveccudaraja.*lib*
	Libraries	libsundials_nveccudampiraja.*lib*
	Header files	nvector/nvector_raja.h
		nvector/nvector_mpiraja.h
		nvector/raja/Vector.hpp
NVECTOR_TRILINOS	Libraries	libsundials_nvectrilinos.*lib*
	Header files	nvector/nvector_trilinos.h
		nvector/trilinos/SundialsTpetraVectorInterface.hpp
		nvector/trilinos/SundialsTpetraVectorKernels.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
		continued on next page

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SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.*lib*
		libsundials_fsunlinsoldense_mod.*lib*
		libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	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
		continued on next page

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SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.*lib* libsundials_fsunlinsolsptfqmr_mod.*lib* libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
	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_impl.h cvode/cvode_direct.h cvode/cvode_ls.h cvode/cvode_spils.h cvode/cvode_bandpre.h cvode/cvode_bbdpre.h
	Module files	fcvode_mod.mod
CVODES	Libraries	libsundials_cvodes.*lib*
	Header files	cvodes/cvodes.h cvodes/cvodes_impl.h cvodes/cvodes_direct.h cvodes/cvodes_ls.h cvodes/cvodes_spils.h cvodes/cvodes_bandpre.h cvodes/cvodes_bbdpre.h
ARKODE	Libraries	libsundials_arkode.*lib* libsundials_farkode.a
	Header files	arkode/arkode.h arkode/arkode_impl.h arkode/arkode_ls.h arkode/arkode_bandpre.h arkode/arkode_bbdpre.h
IDA	Libraries	libsundials_ida.*lib* libsundials_fida.a
	Header files	ida/ida.h ida/ida_impl.h ida/ida_direct.h ida/ida_ls.h ida/ida_spils.h ida/ida_bbdpre.h
IDAS	Libraries	libsundials_idas.*lib*

continued from last page			
	Header files	idas/idas.h	idas/idas_impl.h
		idas/idas_direct.h	idas/idas_ls.h
		idas/idas_spils.h	idas/idas_bbdpre.h
KINSOL	Libraries	libsundials_kinsol.*lib*	libsundials_fkinsol.a
	Header files	kinsol/kinsol.h	kinsol/kinsol_impl.h
		kinsol/kinsol_direct.h	kinsol/kinsol_ls.h
		kinsol/kinsol_spils.h	kinsol/kinsol_bbdpre.h

Appendix B

IDA 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   IDA input constants

	IDA **main solver module**	
`IDA_NORMAL`	1	Solver returns at specified output time.
`IDA_ONE_STEP`	2	Solver returns after each successful step.
`IDA_YA_YDP_INIT`	1	Compute y_a and $\dot{y}_d$, given y_d.
`IDA_Y_INIT`	2	Compute y, given $\dot{y}$.
	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   IDA output constants

	IDA **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 IDA 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.

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.
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.

Bibliography

[1] KLU Sparse Matrix Factorization Library. http://faculty.cse.tamu.edu/davis/suitesparse.html.

[2] SuperLU_DIST Parallel Sparse Matrix Factorization Library. http://crd-legacy.lbl.gov/ xiaoye/-SuperLU/.

[3] SuperLU_MT Threaded Sparse Matrix Factorization Library. http://crd-legacy.lbl.gov/ xiaoye/-SuperLU/.

[4] D. G. Anderson. Iterative procedures for nonlinear integral equations. *J. Assoc. Comput. Machinery*, 12:547–560, 1965.

[5] K. E. Brenan, S. L. Campbell, and L. R. Petzold. *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*. SIAM, Philadelphia, Pa, 1996.

[6] P. N. Brown. A local convergence theory for combined inexact-Newton/finite difference projection methods. *SIAM J. Numer. Anal.*, 24(2):407–434, 1987.

[7] P. N. Brown and A. C. Hindmarsh. Reduced Storage Matrix Methods in Stiff ODE Systems. *J. Appl. Math. & Comp.*, 31:49–91, 1989.

[8] P. N. Brown, A. C. Hindmarsh, and L. R. Petzold. Using Krylov Methods in the Solution of Large-Scale Differential-Algebraic Systems. *SIAM J. Sci. Comput.*, 15:1467–1488, 1994.

[9] P. N. Brown, A. C. Hindmarsh, and L. R. Petzold. Consistent Initial Condition Calculation for Differential-Algebraic Systems. *SIAM J. Sci. Comput.*, 19:1495–1512, 1998.

[10] P. N. Brown and Y. Saad. Hybrid Krylov Methods for Nonlinear Systems of Equations. *SIAM J. Sci. Stat. Comput.*, 11:450–481, 1990.

[11] G. D. Byrne. Pragmatic Experiments with Krylov Methods in the Stiff ODE Setting. In J.R. Cash and I. Gladwell, editors, *Computational Ordinary Differential Equations*, pages 323–356, Oxford, 1992. Oxford University Press.

[12] G. D. Byrne and A. C. Hindmarsh. User Documentation for PVODE, An ODE Solver for Parallel Computers. Technical Report UCRL-ID-130884, LLNL, May 1998.

[13] G. D. Byrne and A. C. Hindmarsh. PVODE, An ODE Solver for Parallel Computers. *Intl. J. High Perf. Comput. Apps.*, 13(4):254–365, 1999.

[14] S. D. Cohen and A. C. Hindmarsh. CVODE, a Stiff/Nonstiff ODE Solver in C. *Computers in Physics*, 10(2):138–143, 1996.

[15] A. M. Collier, A. C. Hindmarsh, R. Serban, and C.S. Woodward. User Documentation for KINSOL v5.0.0-dev.0. Technical Report UCRL-SM-208116, LLNL, 2019.

[16] T. A. Davis and P. N. Ekanathan. Algorithm 907: KLU, a direct sparse solver for circuit simulation problems. *ACM Trans. Math. Softw.*, 37(3), 2010.

[17] R. S. Dembo, S. C. Eisenstat, and T. Steihaug. Inexact Newton Methods. *SIAM J. Numer. Anal.*, 19:400–408, 1982.

[18] J. W. Demmel, J. R. Gilbert, and X. S. Li. An asynchronous parallel supernodal algorithm for sparse gaussian elimination. *SIAM J. Matrix Analysis and Applications*, 20(4):915–952, 1999.

[19] J. E. Dennis and R. B. Schnabel. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*. SIAM, Philadelphia, 1996.

[20] H. Fang and Y. Saad. Two classes of secant methods for nonlinear acceleration. *Numer. Linear Algebra Appl.*, 16:197–221, 2009.

[21] R. W. Freund. A Transpose-Free Quasi-Minimal Residual Algorithm for Non-Hermitian Linear Systems. *SIAM J. Sci. Comp.*, 14:470–482, 1993.

[22] Laura Grigori, James W. Demmel, and Xiaoye S. Li. Parallel symbolic factorization for sparse LU with static pivoting. *SIAM J. Scientific Computing*, 29(3):1289–1314, 2007.

[23] M. R. Hestenes and E. Stiefel. Methods of Conjugate Gradients for Solving Linear Systems. *J. Research of the National Bureau of Standards*, 49(6):409–436, 1952.

[24] K. L. Hiebert and L. F. Shampine. Implicitly Defined Output Points for Solutions of ODEs. Technical Report SAND80-0180, Sandia National Laboratories, February 1980.

[25] A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker, and C. S. Woodward. SUNDIALS, suite of nonlinear and differential/algebraic equation solvers. *ACM Trans. Math. Softw.*, (31):363–396, 2005.

[26] A. C. Hindmarsh and R. Serban. User Documentation for CVODE v5.0.0-dev.0. Technical Report UCRL-SM-208108, LLNL, 2019.

[27] A. C. Hindmarsh, R. Serban, and A. Collier. Example Programs for IDA v5.0.0-dev.0. Technical Report UCRL-SM-208113, LLNL, 2019.

[28] A. C. Hindmarsh, R. Serban, and D. R. Reynolds. Example Programs for CVODE v5.0.0-dev.0. Technical report, LLNL, 2019. UCRL-SM-208110.

[29] A. C. Hindmarsh and A. G. Taylor. PVODE and KINSOL: Parallel Software for Differential and Nonlinear Systems. Technical Report UCRL-ID-129739, LLNL, February 1998.

[30] C. T. Kelley. *Iterative Methods for Solving Linear and Nonlinear Equations*. SIAM, Philadelphia, 1995.

[31] X. S. Li. An overview of SuperLU: Algorithms, implementation, and user interface. *ACM Trans. Math. Softw.*, 31(3):302–325, September 2005.

[32] Xiaoye S. Li and James W. Demmel. SuperLU_DIST: A scalable distributed-memory sparse direct solver for unsymmetric linear systems. *ACM Trans. Mathematical Software*, 29(2):110–140, June 2003.

[33] X.S. Li, J.W. Demmel, J.R. Gilbert, L. Grigori, M. Shao, and I. Yamazaki. SuperLU Users' Guide. Technical Report LBNL-44289, Lawrence Berkeley National Laboratory, September 1999. http://crd.lbl.gov/~xiaoye/SuperLU/. Last update: August 2011.

[34] P. A. Lott, H. F. Walker, C. S. Woodward, and U. M. Yang. An accelerated Picard method for nonlinear systems related to variably saturated flow. *Adv. Wat. Resour.*, 38:92–101, 2012.

[35] Daniel R. Reynolds. Example Programs for ARKODE v4.0.0-dev.0. Technical report, Southern Methodist University, 2019.

[36] Y. Saad. A flexible inner-outer preconditioned GMRES algorithm. *SIAM J. Sci. Comput.*, 14(2):461–469, 1993.

[37] Y. Saad and M. H. Schultz. GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems. *SIAM J. Sci. Stat. Comp.*, 7:856–869, 1986.

[38] H. A. Van Der Vorst. Bi-CGSTAB: A Fast and Smoothly Converging Variant of Bi-CG for the Solution of Nonsymmetric Linear Systems. *SIAM J. Sci. Stat. Comp.*, 13:631–644, 1992.

[39] H. F. Walker and P. Ni. Anderson acceleration for fixed-point iterations. *SIAM Jour. Num. Anal.*, 49(4):1715–1735, 2011.

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