User Documentation for IDA v5.7.0 (SUNDIALS v5.7.0)

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CONTRIBUTORS

The SUNDIALS library has been developed over many years by a number of contributors. The current SUNDIALS team consists of Cody J. Balos, David J. Gardner, Alan C. Hindmarsh, Daniel R. Reynolds, and Carol S. Woodward. We thank Radu Serban for significant and critical past contributions.

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Chapter 1

Introduction

IDA is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [32]. 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 [14, 15], 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 [33, 20] and PVODE [18, 19], and also the nonlinear system solver KINSOL [21].

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) [44], FGMRES (Flexible Generalized Minimum RESidual) [43], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [46], TFQMR (Transpose-Free Quasi-Minimal Residual) [27], and PCG (Preconditioned Conjugate Gradient) [29] 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 v5.7.0

A new NVECTOR implementation based on the SYCL abstraction layer has been added targeting Intel GPUs. At present the only SYCL compiler supported is the DPC++ (Intel oneAPI) compiler. See Section 7.12 for more details. This module is considered experimental and is subject to major changes even in minor releases.

A new SUNMATRIX and SUNLINSOL implementation were added to interface with the MAGMA linear algebra library. Both the matrix and the linear solver support general dense linear systems as well as block diagonal linear systems, and both are targeted at GPUs (AMD or NVIDIA). See Section 9.13 for more details.

Changes in v5.6.1

Fixed a bug in the SUNDIALS CMake which caused an error if the CMAKE_CXX_STANDARD and SUNDIALS_RAJA_BACKENDS options were not provided.

Fixed some compiler warnings when using the IBM XL compilers.

Changes in v5.6.0

A new NVECTOR implementation based on the AMD ROCm HIP platform has been added. This vector can target NVIDIA or AMD GPUs. See 7.10 for more details. This module is considered experimental and is subject to change from version to version.

The RAJA NVECTOR implementation has been updated to support the HIP backend in addition to the CUDA backend. Users can choose the backend when configuring SUNDIALS by using the `SUNDIALS_RAJA_BACKENDS` CMake variable. This module remains experimental and is subject to change from version to version.

A new optional operation, `N_VGetDeviceArrayPointer`, was added to the N_Vector API. This operation is useful for N_Vectors that utilize dual memory spaces, e.g. the native SUNDIALS CUDA N_Vector.

The SUNMATRIX_CUSPARSE and SUNLINEARSOLVER_CUSOLVERSP_BATCHQR implementations no longer require the SUNDIALS CUDA N_Vector. Instead, they require that the vector utilized provides the `N_VGetDeviceArrayPointer` operation, and that the pointer returned by `N_VGetDeviceArrayPointer` is a valid CUDA device pointer.

Changes in v5.5.0

Refactored the SUNDIALS build system. CMake 3.12.0 or newer is now required. Users will likely see deprecation warnings, but otherwise the changes should be fully backwards compatible for almost all users. SUNDIALS now exports CMake targets and installs a SUNDIALSConfig.cmake file.

Added support for SuperLU DIST 6.3.0 or newer.

Changes in v5.4.0

Added the function `IDASetLSNormFactor` to specify the factor for converting between integrator tolerances (WRMS norm) and linear solver tolerances (L2 norm) i.e., `tol_L2 = nrmfac * tol_WRMS`.

The expected behavior of `SUNNonlinSolGetNumIters` and `SUNNonlinSolGetNumConvFails` in the SUNNONLINSOL API have been updated to specify that they should return the number of nonlinear solver iterations and convergence failures in the most recent solve respectively rather than the cumulative number of iterations and failures across all solves respectively. The API documentation and SUNDIALS provided SUNNONLINSOL implementations have been updated accordingly. As before, the cumulative number of nonlinear iterations may be retreived by calling `IDAGetNumNonlinSolvIters`, the cumulative number of failures with `IDAGetNumNonlinSolvConvFails`, or both with `IDAGetNonlinSolvStats`.

A new API, SUNMemoryHelper, was added to support **GPU users** who have complex memory management needs such as using memory pools. This is paired with new constructors for the NVECTOR_CUDA and NVECTOR_RAJA modules that accept a SUNMemoryHelper object. Refer to sections 6.1,11.1, 7.9 and 7.11 for more information.

The NVECTOR_RAJA module has been updated to mirror the NVECTOR_CUDA module. Notably, the update adds managed memory support to the NVECTOR_RAJA module. Users of the module will need to update any calls to the N_VMake_Raja function because that signature was changed. This module remains experimental and is subject to change from version to version.

The NVECTOR_TRILINOS module has been updated to work with Trilinos 12.18+. This update changes the local ordinal type to always be an int.

Added support for CUDA v11.

Changes in v5.3.0

Fixed a bug in the iterative linear solver modules where an error is not returned if the Atimes function is NULL or, if preconditioning is enabled, the PSolve function is NULL.

Added a new function IDAGetNonlinearSystemData which advanced users might find useful if providing a custom SUNNonlinSolSysFn.

Added the ability to control the CUDA kernel launch parameters for the NVECTOR_CUDA and SUNMATRIX_CUSPARSE modules. These modules remain experimental and are subject to change from version to version. In addition, the NVECTOR_CUDA kernels were rewritten to be more flexible. Most users should see equivalent performance or some improvement, but a select few may observe minor performance degradation with the default settings. Users are encouraged to contact the SUNDIALS team about any perfomance changes that they notice.

Added new capabilities for monitoring the solve phase in the SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT modules, and the SUNDIALS iterative linear solver modules. SUNDIALS must be built with the CMake option SUNDIALS_BUILD_WITH_MONITORING to use these capabilties.

Added the optional function IDASetJacTimesResFn to specify an alternative residual function for computing Jacobian-vector products with the internal difference quotient approximation.

Changes in v5.2.0

Fixed a build system bug related to the Fortran 2003 interfaces when using the IBM XL compiler. When building the Fortran 2003 interfaces with an XL compiler it is recommended to set CMAKE_Fortran_COMPILER to f2003, xlf2003, or xlf2003_r.

Fixed a linkage bug affecting Windows users that stemmed from dllimport/dllexport attributes missing on some SUNDIALS API functions.

Added a new SUNMatrix implementation, SUNMATRIX_CUSPARSE, that interfaces to the sparse matrix implementation from the NVIDIA cuSPARSE library. In addition, the SUNLINSOL_CUSOLVER_BATCHQR linear solver has been updated to use this matrix, therefore, users of this module will need to update their code. These modules are still considered to be experimental, thus they are subject to breaking changes even in minor releases.

The function IDASetLinearSolutionScaling was added to enable or disable the scaling applied to linear system solutions with matrix-based linear solvers to account for a lagged value of α in the linear system matrix $\frac{\partial F}{\partial y} + \alpha \frac{\partial F}{\partial \dot{y}}$. Scaling is enabled by default when using a matrix-based linear solver.

Changes in v5.1.0

Fixed a build system bug related to finding LAPACK/BLAS.

Fixed a build system bug related to checking if the KLU library works.

Fixed a build system bug related to finding PETSc when using the CMake variables PETSC_INCLUDES and PETSC_LIBRARIES instead of PETSC_DIR.

Added a new build system option, CUDA_ARCH, that can be used to specify the CUDA architecture to compile for.

Added two utility functions, `SUNDIALSFileOpen` and `SUNDIALSFileClose` for creating/destroying file pointers that are useful when using the Fortran 2003 interfaces.

Changes in v5.0.0

Build system changes

- Increased the minimum required CMake version to 3.5 for most SUNDIALS configurations, and 3.10 when CUDA or OpenMP with device offloading are enabled.
- The CMake option `BLAS_ENABLE` and the variable `BLAS_LIBRARIES` have been removed to simplify builds as SUNDIALS packages do not use BLAS directly. For third party libraries that require linking to BLAS, the path to the BLAS library should be included in the `_LIBRARIES` variable for the third party library *e.g.*, `SUPERLUDIST_LIBRARIES` when enabling SuperLU_DIST.
- Fixed a bug in the build system that prevented the NVECTOR_PTHREADS module from being built.

NVECTOR module changes

- Two new functions were added to aid in creating custom NVECTOR objects. The constructor `N_VNewEmpty` allocates an "empty" generic NVECTOR with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the NVECTOR API by ensuring only required operations need to be set. Additionally, the function `N_VCopyOps(w, v)` has been added to copy the operation function pointers between vector objects. When used in clone routines for custom vector objects these functions also will ease the introduction of any new optional operations to the NVECTOR API by ensuring all operations are copied when cloning objects. See §7.1.6 for more details.
- Two new NVECTOR implementations, NVECTOR_MANYVECTOR and NVECTOR_MPIMANYVECTOR, have been 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. This implementation is accompanied by additions to user documentation and SUNDIALS examples. See §7.15 and §7.16 for more details.
- One new required vector operation and ten new optional vector operations have been added to the NVECTOR API. The new required operation, `N_VGetLength`, returns the global length of an `N_Vector`. The optional operations have been added to support the new NVECTOR_MPIMANYVECTOR implementation. The operation `N_VGetCommunicator` must be implemented by subvectors that are combined to create an NVECTOR_MPIMANYVECTOR, but is 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_MPIMANYVECTOR will call standard NVECTOR operations to complete the computation. See §7.1.4 for more details.
- An additional NVECTOR implementation, NVECTOR_MPIPLUSX, has been created to support the MPI+X paradigm where X is a type of on-node parallelism (*e.g.*, OpenMP, CUDA). The implementation is accompanied by additions to user documentation and SUNDIALS examples. See §7.17 for more details.
- The `*_MPICuda` and `*_MPIRaja` functions have been removed from the NVECTOR_CUDA and NVECTOR_RAJA implementations respectively. Accordingly, the `nvector_mpicuda.h`,

`nvector_mpiraja.h`, `libsundials_nvecmpicuda.lib`, and `libsundials_nvecmpicudaraja.lib` files have been removed. Users should use the NVECTOR_MPIPLUSX module coupled in conjunction with the NVECTOR_CUDA or NVECTOR_RAJA modules to replace the functionality. The necessary changes are minimal and should require few code modifications. See the programs in `examples/ida/mpicuda` and `examples/ida/mpiraja` for examples of how to use the NVECTOR_MPIPLUSX module with the NVECTOR_CUDA and NVECTOR_RAJA modules respectively.

- Fixed a memory leak in the NVECTOR_PETSC module clone function.
- Made performance improvements to the NVECTOR_CUDA module. Users who utilize a non-default stream should no longer see default stream synchronizations after memory transfers.
- Added a new constructor to the NVECTOR_CUDA module that allows a user to provide custom allocate and free functions for the vector data array and internal reduction buffer. See §7.9.1 for more details.
- Added new Fortran 2003 interfaces for most NVECTOR modules. See Chapter 7 for more details on how to use the interfaces.
- Added three new NVECTOR utility functions, `FN_VGetVecAtIndexVectorArray`, `FN_VSetVecAtIndexVectorArray`, and `FN_VNewVectorArray`, for working with `N_Vector` arrays when using the Fortran 2003 interfaces. See §7.1.6 for more details.

SUNMatrix module changes

- Two new functions were added to aid in creating custom SUNMATRIX objects. The constructor `SUNMatNewEmpty` allocates an "empty" generic SUNMATRIX with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the SUNMATRIX API by ensuring only required operations need to be set. Additionally, the function `SUNMatCopyOps(A, B)` has been added to copy the operation function pointers between matrix objects. When used in clone routines for custom matrix objects these functions also will ease the introduction of any new optional operations to the SUNMATRIX API by ensuring all operations are copied when cloning objects. See §8.1.2 for more details.
- A new operation, `SUNMatMatvecSetup`, was added to the SUNMATRIX API to perform any setup necessary for computing a matrix-vector product. This operation is useful for SUNMATRIX implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product. 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`. See §8.1.1 for more details.
- 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. See §8.1.3 for more details.
- A new SUNMATRIX (and SUNLINSOL) implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS. See §8.6 for more details.
- Added new Fortran 2003 interfaces for most SUNMATRIX modules. See Chapter 8 for more details on how to use the interfaces.

SUNLinearSolver module changes

- A new function was added to aid in creating custom SUNLINSOL objects. The constructor `SUNLinSolNewEmpty` allocates an "empty" generic SUNLINSOL with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional

operations to the SUNLINSOL API by ensuring only required operations need to be set. See §9.3 for more details.

- The return type of the SUNLINSOL API function `SUNLinSolLastFlag` has changed from `long int` to `sunindextype` to be consistent with the type used to store row indices in dense and banded linear solver modules.
- Added a new optional operation to the SUNLINSOL API, `SUNLinSolGetID`, that returns a `SUNLinearSolver_ID` for identifying the linear solver module.
- The SUNLINSOL API has been updated to make the initialize and setup functions optional.
- A new SUNLINSOL (and SUNMATRIX) implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS. See §9.10 for more details.
- Added a new SUNLINSOL implementation, `SUNLinearSolver_cuSolverSp_batchQR`, which leverages the NVIDIA cuSOLVER sparse batched QR method for efficiently solving block diagonal linear systems on NVIDIA GPUs. See §9.12 for more details.
- Added three new accessor functions to the SUNLINSOL_KLU module, `SUNLinSol_KLUGetSymbolic`, `SUNLinSol_KLUGetNumeric`, and `SUNLinSol_KLUGetCommon`, to provide user access to the underlying KLU solver structures. See §9.9.2 for more details.
- Added new Fortran 2003 interfaces for most SUNLINSOL modules. See Chapter 9 for more details on how to use the interfaces.

SUNNonlinearSolver module changes

- A new function was added to aid in creating custom SUNNONLINSOL objects. The constructor `SUNNonlinSolNewEmpty` allocates an "empty" generic SUNNONLINSOL with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the SUNNONLINSOL API by ensuring only required operations need to be set. See §10.1.8 for more details.
- To facilitate the use of user supplied nonlinear solver convergence test functions the `SUNNonlinSolSetConvTestFn` function in the SUNNONLINSOL API has been updated to take a `void*` data pointer as input. The supplied data pointer will be passed to the nonlinear solver convergence test function on each call.
- The inputs values passed to the first two inputs of the `SUNNonlinSolSolve` function in the SUNNONLINSOL have been changed to be the predicted state and the initial guess for the correction to that state. Additionally, the definitions of `SUNNonlinSolLSetupFn` and `SUNNonlinSolLSolveFn` in the SUNNONLINSOL API have been updated to remove unused input parameters. For more information on the nonlinear system formulation see §10.2 and for more details on the API functions see Chapter 10.
- Added a new SUNNONLINSOL implementation, SUNNONLINSOL_PETSCSNES, which interfaces to the PETSc SNES nonlinear solver API. See §10.4 for more details.
- Added new Fortran 2003 interfaces for most SUNNONLINSOL modules. See Chapter 10 for more details on how to use the interfaces.

IDA changes

- A bug was fixed in the IDA linear solver interface where an incorrect Jacobian-vector product increment was used with iterative solvers other than SUNLINSOL_SPGMR and SUNLINSOL_SPFGMR.
- Fixed a memeory leak in FIDA when not using the default nonlinear solver.

- Removed extraneous calls to `N_VMin` for simulations where the scalar valued absolute tolerance, or all entries of the vector-valued absolute tolerance array, are strictly positive. In this scenario, IDA will remove at least one global reduction per time step.
- The IDALS interface has been updated to only zero the Jacobian matrix before calling a user-supplied Jacobian evaluation function when the attached linear solver has type `SUNLINEARSOLVER_DIRECT`.
- Added the new functions, `IDAGetCurentCj`, `IDAGetCurrentY`, `IDAGetCurrentYp`, `IDAComputeCurrentY`, and `IDAComputeCurrentYp` which may be useful to users who choose to provide their own nonlinear solver implementations.
- Added a Fortran 2003 interface to IDA. See Chapter 5 for more details.

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 9. 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 10 and follow the same object oriented design and implementation used by the NVECTOR, SUNMATRIX, and SUNLINSOL modules. Currently two SUNNONLINSOL implementations are provided, SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT. These replicate the previous integrator specific implementations of a Newton iteration and a fixed-point iteration (previously referred to as a functional iteration), respectively. Note the SUNNONLINSOL_FIXEDPOINT module can optionally utilize Anderson's method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all 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 SUNNONLINSOL_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 7 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 §7.13 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 depreated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPI_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.
- When a Fortran name-mangling scheme is needed (e.g., `ENABLE_LAPACK` 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 SUNDIALS_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 5.2).

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 5.2, we describe FIDA, an interface module for the use of IDA with FORTRAN applications.
- Chapter 7 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 8 gives a brief overview of the generic SUNMATRIX module shared among the various components of SUNDIALS, and details on the SUNMATRIX implementations provided with SUNDIALS: a dense implementation (§8.3), a banded implementation (§8.4) and a sparse implementation (§8.5).
- Chapter 9 gives a brief overview of the generic SUNLINSOL module shared among the various components of SUNDIALS. This chapter contains details on the SUNLINSOL implementations provided with SUNDIALS. The chapter also contains details on the SUNLINSOL implementations provided with SUNDIALS that interface with external linear solver libraries.
- Chapter 10 describes the SUNNONLINSOL API and nonlinear solver implementations shared among the various components of SUNDIALS.
- Finally, in the appendices, we provide detailed instructions for the installation of 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.

1.3 SUNDIALS Release License

All SUNDIALS packages are released open source, under the BSD 3-Clause license. The only requirements of the license are preservation of copyright and a standard disclaimer of liability. The full text of the license and an additional notice are provided below and may also be found in the LICENSE and NOTICE files provided with all SUNDIALS packages.

If you are using SUNDIALS with any third party libraries linked in (e.g., LAPACK, KLU, SuperLU_MT, PETSc, or *hypre*), be sure to review the respective license of the package as that license may have more restrictive terms than the SUNDIALS license. For example, if someone builds SUNDIALS with a statically linked KLU, the build is subject to terms of the LGPL license (which is what KLU is released with) and *not* the SUNDIALS BSD license anymore.

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1.3.2 Additional Notice

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 [15]. 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 [11]. 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 10). 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 9). The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- band direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- sparse direct solver interfaces, using either the KLU sparse solver library [22, 3], or the thread-enabled SuperLU_MT sparse solver library [39, 24, 9] (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 [13]. 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 $\|\cdot\|_{\mathrm{WRMS}}$, for all error-like quantities. The multiplicative weights used are based on the current solution and on the relative and absolute tolerances input by the user, namely

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

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

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

where U is the unit roundoff, h is the current step size, and W_j is the error weight for the component y_j defined by (2.6). 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 $\sigma = 1/\|v\|$. 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:

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

The value of η is adjusted such that (a) if $\eta > 2$, η is reset to 2; (b) if $\eta \leq 1$, η is restricted to $0.5 \leq \eta \leq 0.9$; and (c) if $1 < \eta < 2$ we use $\eta = 1$. Finally h is reset to $h' = \eta h$. Thus we do not increase the step size unless it can be doubled. See [11] 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. If a step fails to satisfy the constraints repeatedly within a step attempt then the integration is halted and an error is returned. In this case the user may need to employ other strategies as discussed in §4.5.2 to satisfy the inequality constraints.

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

2.2 Preconditioning

When using a nonlinear solver that requires the solution of a linear system of the form $J\Delta y = -G$ (e.g., the default Newton iteration), 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 [13] 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 [30]. 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 $t_{\rm out}$ if this comes sooner. The endpoint t_{lo} is either t_{n-1}, or the last output time $t_{\rm out}$ (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 Figures 3.1 and 3.2). The

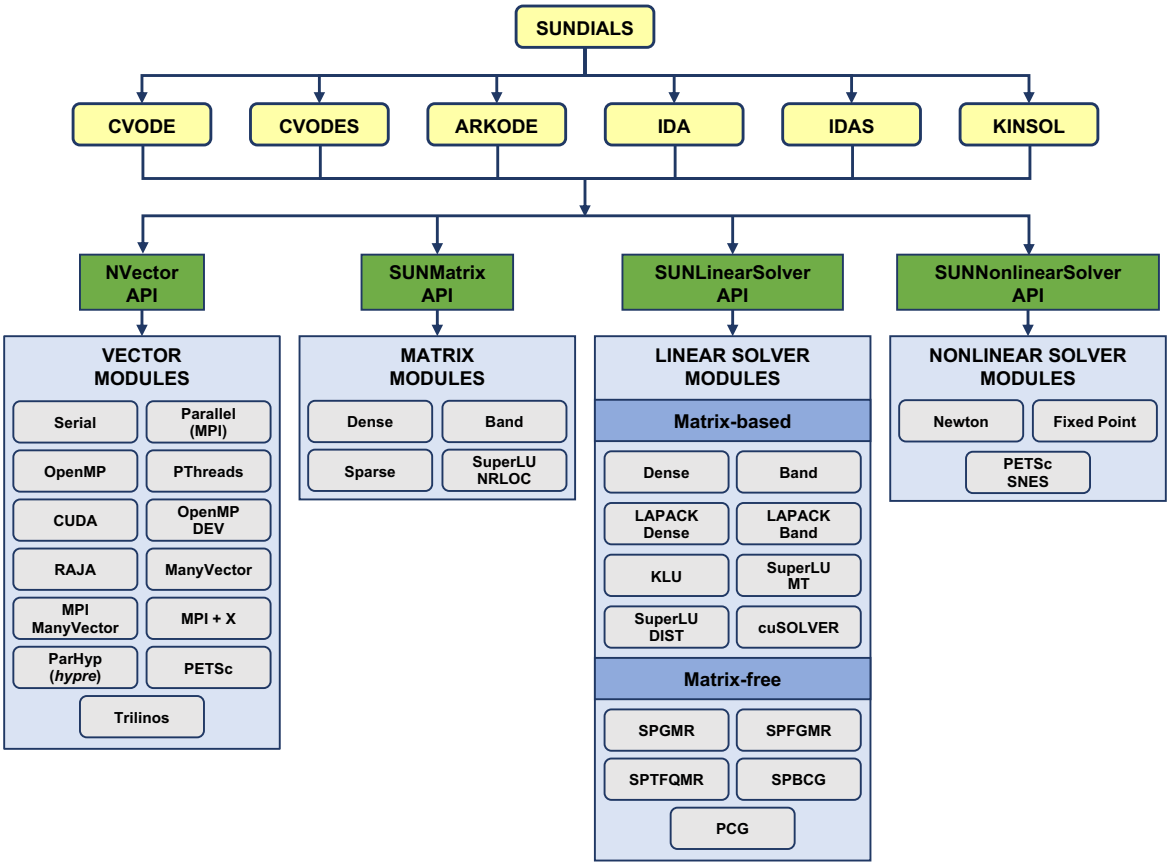

Figure 3.1: High-level diagram of the SUNDIALS suite.

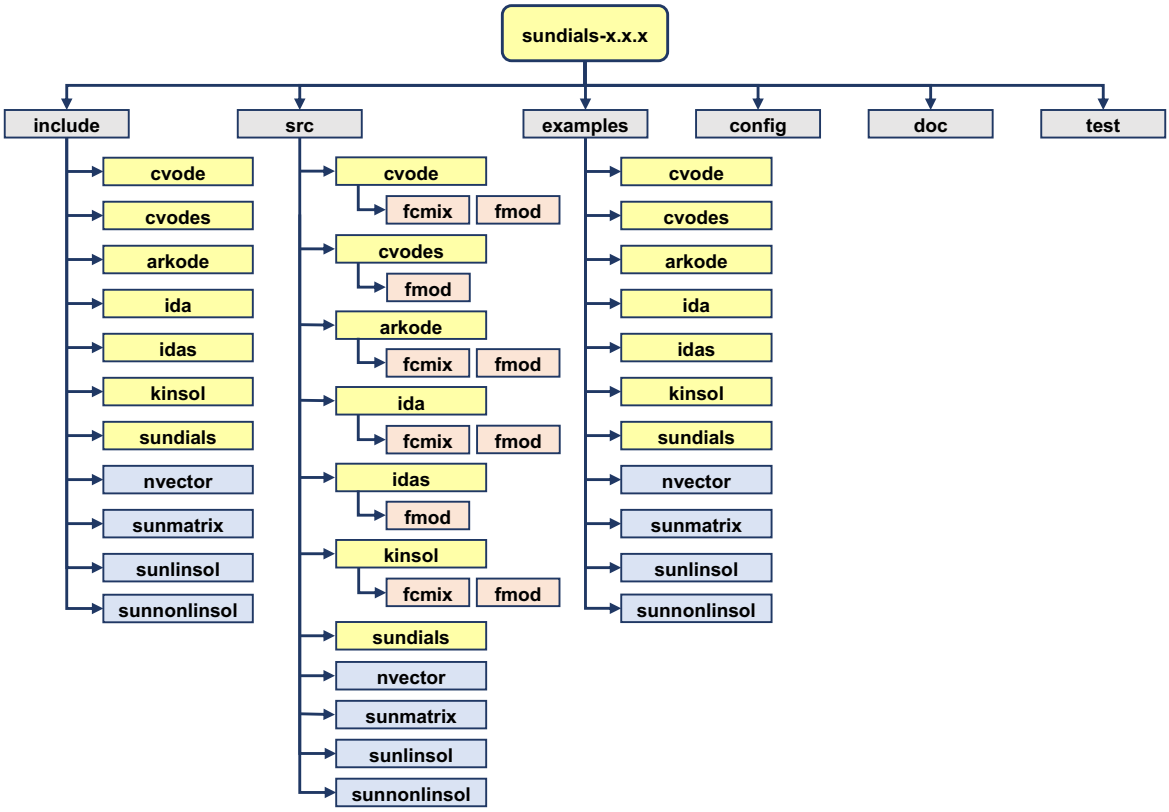

Figure 3.2: Directory structure of the SUNDIALS source tree.

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 stiff, nonstiff, mixed stiff-nonstiff, and multirate ODE systems $M dy/dt = f_1(t, y) + f_2(t, y)$ based on 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 $F(u) = 0$.

Note for modules that provide interfaces to third-party libraries (i.e., LAPACK, KLU, SUPERLUMT, SuperLU_DIST, *hypre*, PETSc, Trilinos, and RAJA) users will need to download and compile those packages independently.

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

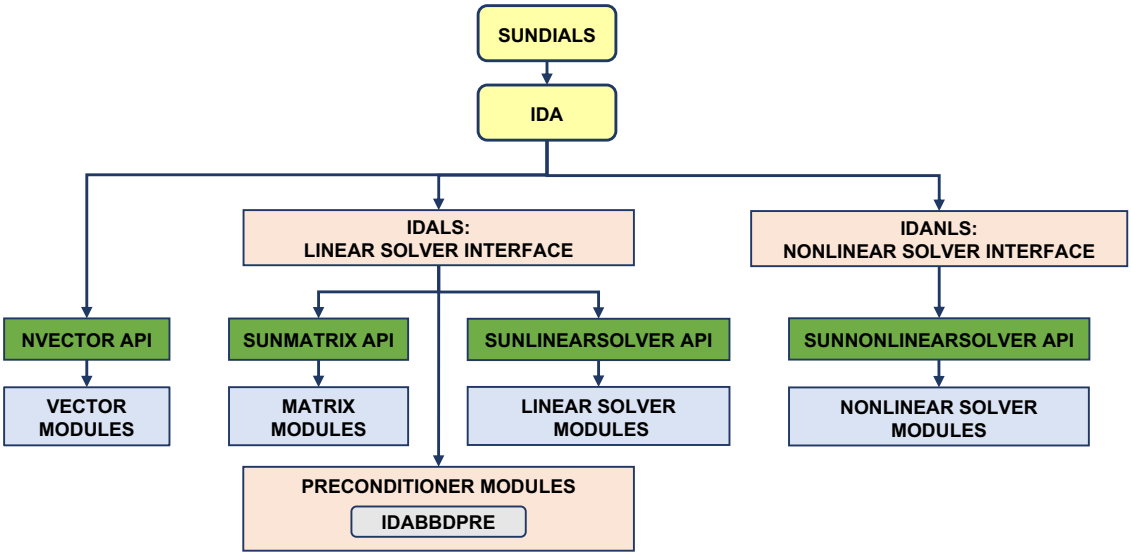

Figure 3.3: Overall structure diagram of the IDA package. Modules specific to IDA begin with "IDA" (IDALS, IDANLS, and IDABBDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver modules (see Figure 3.1).

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 9) and SUNNONLINSOL API (see Chapter 10) 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 9). These solvers may utilize a SUNMATRIX object (see Chapter 8) 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 [13, 17], 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 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 [34] 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 5.2, 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 8) and each SUNLINSOL module (Chapter 9). For example, NVECTOR_PARALLEL is not compatible with the dense, banded, or sparse SUNMATRIX types, or with the corresponding dense, banded, or sparse SUNLINSOL modules. Please check Chapters 8 and 9 to verify compatibility between these modules. In addition to that documentation, we note that the preconditioner module IDABBDPRE can only be used with NVECTOR_PARALLEL. It is not recommended to use a threaded vector module with SuperLU_MT unless it is the NVECTOR_OPENMP module, and SuperLU_MT is also compiled with OpenMP.

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.

Additionally, SUNDIALS defines several macros for common mathematical functions *e.g.*, fabs, sqrt, exp, etc. in sundials_math.h. The macros are prefixed with SUNR and expand to the appropriate C function based on the realtype. For example, the macro SUNRabs expands to the C function fabs when realtype is double, fabsf when realtype is float, and fabsl when realtype is long double.

A user program which uses the type realtype, the RCONST macro, and the SUNR mathematical function macros is precision-independent except for any calls to precision-specific library functions. Our example programs use realtype, RCONST, and the SUNR macros. 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) and call the appropriate math library functions directly. Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use realtype, RCONST, or the SUNR macros so long as the SUNDIALS libraries use the correct precision (for details see §A.1.2).

4.2.2 Integer types used for indexing

The type `sunindextype` is used for indexing array entries in SUNDIALS modules (*e.g.*, vectors lengths and matrix sizes) as well as for storing the total problem size. During configuration `sunindextype` may be selected to be either a 32- or 64-bit *signed* integer with the default being 64-bit. See §A.1.2 for the configuration option to select the desired size of `sunindextype`. When using a 32-bit integer the total problem size is limited to $2^{31}-1$ and with 64-bit integers the limit is $2^{63}-1$. For users with problem sizes that exceed the 64-bit limit an advanced configuration option is available to specify the type used for `sunindextype`.

A user program which uses `sunindextype` to handle 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 compatible type (*e.g.*, `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 7 for the appropriate name. This file in turn includes the header file `sundials_nvector.h` which defines the abstract `N_Vector` data type.

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

If using a nonlinear solver that requires the solution of a linear system of the form (2.4) (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, SUNLINSOL_DENSE;
  - `sunlinsol/sunlinsol_band.h`, which is used with the banded linear solver module, SUNLINSOL_BAND;
  - `sunlinsol/sunlinsol_lapackdense.h`, which is used with the LAPACK dense linear solver module, SUNLINSOL_LAPACKDENSE;
  - `sunlinsol/sunlinsol_lapackband.h`, which is used with the LAPACK banded linear solver module, SUNLINSOL_LAPACKBAND;
  - `sunlinsol/sunlinsol_klu.h`, which is used with the KLU sparse linear solver module, SUNLINSOL_KLU;
  - `sunlinsol/sunlinsol_superlumt.h`, which is used with the SUPERLUMT sparse linear solver module, SUNLINSOL_SUPERLUMT;

- Iterative linear solvers:
  - `sunlinsol/sunlinsol_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver module, SUNLINSOL_SPGMR;
  - `sunlinsol/sunlinsol_spfgmr.h`, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, SUNLINSOL_SPFGMR;
  - `sunlinsol/sunlinsol_spbcgs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, SUNLINSOL_SPBCGS;
  - `sunlinsol/sunlinsol_sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov linear solver module, SUNLINSOL_SPTFQMR;
  - `sunlinsol/sunlinsol_pcg.h`, which is used with the scaled, preconditioned CG Krylov linear solver module, SUNLINSOL_PCG;

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

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

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

The header files for the Krylov iterative solvers include the file `sundials/sundials_iterative.h`, which enumerates the kind of preconditioning, and (for the SPGMR and SPFGMR solvers) the choices for the Gram-Schmidt process.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the `idaFoodWeb_kry_p` example (see [34]), preconditioning is done with a block-diagonal matrix. For this, even though the SUNLINSOL_SPGMR linear solver is used, the header `sundials/sundials_dense.h` is included for access to the underlying generic dense matrix arithmetic routines.

4.4 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the integration of a DAE IVP. Most of the steps are independent of the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapter 7, 8, 9, and 10 for the specific name of the function to be called or macro to be referenced.

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

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

2. **Set problem dimensions etc.**

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

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

3. **Set vectors of initial values**

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

   For native SUNDIALS vector implementations, use a call of the form `y0 = N_VMake_***(..., ydata)` if the `realtype` array `ydata` containing the initial values of y already exists. Otherwise, create a new vector by making a call of the form `y0 = N_VNew_***(...)`, and then set its elements

by accessing the underlying data with a call of the form `ydata = N_VGetArrayPointer(y0)`. See §7.3-7.6 for details.

For the *hypre* and PETSc vector wrappers, first create and initialize the underlying vector and then create an NVECTOR wrapper with a call of the form `y0 = N_VMake_***(yvec)`, where `yvec` is a *hypre* or PETSc vector. Note that calls like `N_VNew_***(...)` and `N_VGetArrayPointer(...)` are not available for these vector wrappers. See §7.7 and §7.8 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 9.

9. **Set linear solver optional inputs**

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

10. **Attach linear solver module**

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

    ```
    ier = IDASetLinearSolver(...);
    ```

11. **Set optional inputs**

    Optionally, call `IDASet*` functions to change from their default values any optional inputs that control the behavior of 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 implementation (e.g., `NLS = SUNNonlinSol_***(...);` where `***` is the name of the nonlinear solver (see Chapter 10 for details).

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

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

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

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

15. **Correct initial values**

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

16. **Specify rootfinding problem**

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

17. **Advance solution in time**

    For each point at which output is desired, call `flag = IDASolve(ida_mem, tout, &tret, yret, ypret, itask)`. Here `itask` specifies the return mode. The vector `yret` (which can be the same as the vector `y0` above) will contain $y(t)$, while the vector `ypret` (which can be the same as the vector `yp0` above) will contain $\dot{y}(t)$. See §4.5.7 for details.

18. **Get optional outputs**

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

19. **Deallocate memory for solution vectors**

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

`N_VDestroy(yret);`

and similarly for `ypret`.

20. **Free solver memory**

    `IDAFree(&ida_mem)` to free the memory allocated for 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 9 the SUNDIALS packages operate on generic SUNLINSOL objects, allowing a user to develop their own solvers should they so desire.

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

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

4.5 User-callable functions

This section describes the 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`.

F2003 Name `FIDACreate`

`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.

F2003 Name `FIDAInit`

`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.

F2003 Name `FIDAFree`

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.

F2003 Name `FIDASStolerances`

`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.

F2003 Name `FIDASVtolerances`

`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.

F2003 Name `FIDAWFtolerances`

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 [34]. 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, if the nonlinear solver requires the solution of linear systems of the form (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 8 and 9.

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 8 for further information).

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

F2003 Name FIDASetLinearSolver

4.5.4 Nonlinear solver interface function

By default IDA uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §10.3). 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.

F2003 Name FIDASetNonlinearSolver

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. [15].) 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).

F2003 Name FIDACalcIC

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`$= 0$.

F2003 Name `FIDARootInit`

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(`tout`) and $\dot{y}$(`tout`). The `IDA_ONE_STEP` option tells the solver to just take one internal step and return the solution at the point reached by that step.

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

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

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

IDA_SUCCESS	IDASolve succeeded.
IDA_TSTOP_RETURN	IDASolve succeeded by reaching the stop point specified through the optional input function IDASetStopTime. 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.

F2003 Name FIDASolve

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 of the optional input functions also send an error message to the error handler function. All error return values are negative, so the test `flag < 0` will catch all errors. Finally, a call to a `IDASet***` function can be made from the user's calling program at any time and, if successful, takes effect immediately.

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);`

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.

F2003 Name `FIDASetErrFile`

`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`.

F2003 Name `FIDASetErrHandlerFn`

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
Enable or disable linear solution scaling	`IDASetLinearSolutionScaling`	on
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
Jacobian-times-vector DQ Res function	`IDASetJacTimesResFn`	NULL
Newton linear solve tolerance conversion factor	`IDASetLSNormFactor`	vector length

`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.

F2003 Name `FIDASetUserData`

`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.

F2003 Name `FIDASetMaxOrd`

`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).*

F2003 Name `FIDASetMaxNumSteps`

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

F2003 Name `FIDASetInitStep`

`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 ∞.

F2003 Name `FIDASetMaxStep`

`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`).

F2003 Name `FIDASetStopTime`

`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.

F2003 Name `FIDASetMaxErrTestFails`

`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.

F2003 Name `FIDASetMaxNonlinIters`

`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.

F2003 Name `FIDASetMaxConvFails`

`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.

F2003 Name `FIDASetNonlinConvCoef`

`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. [11] for more on this issue.

F2003 Name `FIDASetSuppressAlg`

`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).

F2003 Name `FIDASetId`

`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

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

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

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

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

F2003 Name `FIDASetConstraints`

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.

F2003 Name `FIDASetJacFn`

When using a matrix-based linear solver the matrix information will be updated infrequently to reduce matrix construction and, with direct solvers, factorization costs. As a result the value of α may not be current and a scaling factor is applied to the solution of the linear system to account for the lagged value of α. See §9.4.1 for more details. The function `IDASetLinearSolutionScaling` can be used to disable this scaling when necessary, e.g., when providing a custom linear solver that updates the matrix using the current α as part of the solve.

`IDASetLinearSolutionScaling`

Call `flag = IDASetLinearSolutionScaling(ida_mem, onoff);`

Description The function `IDASetLinearSolutionScaling` enables or disables scaling the linear system solution to account for a change in α in the linear system. For more details see §9.4.1.

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

`onoff` (`booleantype`) flag to enable (`SUNTRUE`) or disable (`SUNFALSE`) scaling

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

`IDALS_SUCCESS`	The flag 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.
`IDALS_ILL_INPUT`	The attached linear solver is not matrix-based.

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

By default scaling is enabled with matrix-based linear solvers.

F2003 Name `FIDASetLinearSolutionScaling`

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.

F2003 Name `FIDASetJacTimes`

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.

F2003 Name `FIDASetIncrementFactor`

Additionally, when using the internal difference quotient, the user may also optionally supply an alternative residual function for use in the Jacobian-vector product approximation by calling `IDASetJacTimesResFn`. The alternative residual function should compute a suitable (and differentiable) approximation to the residual function provided to `IDAInit`. For example, as done in [26] for an ODE in explicit form, the alternative function may use lagged values when evaluating a nonlinearity to avoid differencing a potentially non-differentiable factor.

`IDASetJacTimesResFn`

Call `flag = IDASetJacTimesResFn(ida_mem, jtimesResFn);`

Description The function `IDASetJacTimesResFn` specifies an alternative DAE residual function for use in the internal Jacobian-vector product difference quotient approximation.

Arguments
- `ida_mem` (`void *`) pointer to the IDA memory block.
- `jtimesResFn` (`IDAResFn`) is the C function which computes the alternative DAE residual function to use in Jacobian-vector product difference quotient approximations. This function has the form `res(t, yy, yp, resval, user_data)`. For full details see §4.6.1.

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 internal difference quotient approximation is disabled.

Notes The default is to use the residual function provided to `IDAInit` in the internal difference quotient. If the input resudual function is `NULL`, the default is used.

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

F2003 Name `FIDASetJacTimesResFn`

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.

F2003 Name `FIDASetPreconditioner`

`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.

F2003 Name `FIDASetEpsLin`

IDASetLSNormFactor

Call `flag = IDASetLSNormFactor(ida_mem, nrmfac);`

Description The function `IDASetLSNormFactor` specifies the factor to use when converting from the integrator tolerance (WRMS norm) to the linear solver tolerance (L2 norm) for Newton linear system solves e.g., `tol_L2 = fac * tol_WRMS`.

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

`nrmfac` (`realtype`) the norm conversion factor. If `nrmfac` is:

- > 0 then the provided value is used.
- $= 0$ then the conversion factor is computed using the vector length i.e., `nrmfac = N_VGetLength(y)` (*default*).
- < 0 then the conversion factor is computed using the vector dot product `nrmfac = N_VDotProd(v,v)` where all the entries of `v` are one.

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

Prior to the introduction of `N_VGetLength` in SUNDIALS v5.0.0 (IDA v5.0.0) the value of `nrmfac` was computed using the vector dot product i.e., the `nrmfac < 0` case.

F2003 Name `FIDASetLSNormFactor`

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.

F2003 Name `FIDASetNonlinConvCoefIC`

`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.

F2003 Name `FIDASetMaxNumStepsIC`

`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.

F2003 Name `FIDASetMaxNumJacsIC`

`IDASetMaxNumItersIC`

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

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

Arguments `ida_mem` (`void *`) pointer to the 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.

F2003 Name `FIDASetMaxNumItersIC`

`IDASetMaxBacksIC`

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

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

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`maxbacks` (`int`) maximum number of linesearch backtracks per Newton step.

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

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

Notes The default value is 100.

F2003 Name `FIDASetMaxBacksIC`

`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`.

F2003 Name `FIDASetLineSearchOffIC`

`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)$^{2/3}$.

F2003 Name `FIDASetStepToleranceIC`

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.

F2003 Name `FIDASetRootDirection`

`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.

F2003 Name `FIDASetNoInactiveRootWarn`

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 k^{th} 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 $klast$.

F2003 Name `FIDAGetDky`

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 information.

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

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

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

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

`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, additional extraction functions provide the optional outputs in groups. These optional output functions are described next.

`IDAGetWorkSpace`

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

Description The function `IDAGetWorkSpace` returns the 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 $m = \max($`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.

F2003 Name `FIDAGetWorkSpace`

`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`.

F2003 Name `FIDAGetNumSteps`

`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.

F2003 Name `FIDAGetNumResEvals`

`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`.

F2003 Name `FIDAGetNumLinSolvSetups`

`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`.

F2003 Name `FIDAGetNumErrTestFails`

`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`.

F2003 Name `FIDAGetLastOrder`

`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`.

F2003 Name `FIDAGetCurrentOrder`

`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`.

F2003 Name `FIDAGetLastStep`

`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`.

F2003 Name `FIDAGetCurrentStep`

`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 ($h_{\min} \le h_0 \le h_{\max}$), or to meet the local error test.

F2003 Name `FIDAGetActualInitStep`

`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`.

F2003 Name `FIDAGetCurrentTime`

`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`.

F2003 Name `FIDAGetTolScaleFactor`

`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`.

F2003 Name `FIDAGetErrWeights`

`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]`.

F2003 Name `FIDAGetEstLocalErrors`

`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`.

F2003 Name `FIDAGetIntegratorStats`

`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`.

F2003 Name `FIDAGetNumNonlinSolvIters`

`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`.

F2003 Name `FIDAGetNumNonlinSolvConvFails`

`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.

F2003 Name FIDAGetNonlinSolvStats

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.

F2003 Name FIDAGetReturnFlagName

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.

F2003 Name FIDAGetNumBcktrackOps

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).

F2003 Name FIDAGetConsistentIC

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`.

F2003 Name `FIDAGetRootInfo`

`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`.

F2003 Name `FIDAGetNumGEvals`

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.

F2003 Name FIDAGetLinWorkSpace

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.

F2003 Name FIDAGetNumJacEvals

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.

F2003 Name FIDAGetNumLinResEvals

`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.

F2003 Name `FIDAGetNumLinIters`

`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.

F2003 Name `FIDAGetNumLinConvFails`

`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.

F2003 Name `FIDAGetNumPrecEvals`

`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.

F2003 Name `FIDAGetNumPrecSolves`

`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.

F2003 Name `FIDAGetNumJTSetupEvals`

`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.

F2003 Name `FIDAGetNumJtimesEvals`

`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.

F2003 Name `FIDAGetLastLinFlag`

`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.

F2003 Name `FIDAGetLinReturnFlagName`

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 function.

F2003 Name `FIDAReInit`

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 solution of the nonlinear solver. Therefore, in general, a recoverable error in that converged value cannot be corrected. (It may be detected when the residual 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 $\| v\|_{\text{WRMS}} = \sqrt{(1/N)\sum_1^N (W_i \cdot v_i)^2}$. These weights will used in place of those defined by Eq. (2.6). 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,
                         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,
                          N_Vector yy, N_Vector yp, N_Vector rr,
                          SUNMatrix Jac, void *user_data,
                          N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the Jacobian matrix J of the DAE system (or an approximation to it), defined by Eq. (2.5).

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 (α 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 α 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 8 for details).

With direct linear solvers (i.e., linear solvers with type `SUNLINEARSOLVER_DIRECT`), the Jacobian matrix $J(t, y)$ is zeroed out prior to calling the user-supplied Jacobian function so only nonzero elements need to be loaded into `Jac`.

With the default nonlinear solver (the native SUNDIALS Netwon method), each call to the user's `IDALsJacFn` function is preceded by a call to the `IDAResFn` user function with the same (`tt`, `yy`, `yp`) arguments. Thus the Jacobian function can use any auxiliary data that is computed and saved during the evaluation of the DAE residual. In the case of a user-supplied or external nonlinear solver, this is also true if the residual function is evaluated prior to calling the linear solver setup function (see §10.1.4 for more information).

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 ... 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 ... N − 1), and the elements of the j-th column can then be accessed using ordinary array indexing. Consequently, $J_{m,n}$ can be loaded using the statements col_n = SM_COLUMN_D(J, n-1); col_n[m-1] = $J_{m,n}$. For large problems, it is more efficient to use SM_COLUMN_D than to use SM_ELEMENT_D. Note that both of these macros number rows and columns starting from 0. The SUNMATRIX_DENSE type and accessor macros are documented in §8.3.

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 ≤ m-n ≤ mlower. Alternatively, SM_COLUMN_B(J, j) returns a pointer to the diagonal element of the j-th column of Jac, and if we assign this address to realtype *col_j, then the i-th element of the j-th column is given by SM_COLUMN_ELEMENT_B(col_j, i, j), counting from 0. Thus, for (m, n) within the band, $J_{m,n}$ can be loaded by setting col_n = SM_COLUMN_B(J, n-1); and SM_COLUMN_ELEMENT_B(col_n, m-1, n-1) = $J_{m,n}$. The elements of the j-th column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type SUNMATRIX_BAND. The array col_n can be indexed from −mupper to mlower. For large problems, it is more efficient to use SM_COLUMN_B and SM_COLUMN_ELEMENT_B than to use the SM_ELEMENT_B macro. As in the dense case, these macros all number rows and columns starting from 0. The SUNMATRIX_BAND type and accessor macros are documented in §8.4.

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 documented in §8.5.

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

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

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

IDALsJacTimesVecFn

Definition
```
typedef int (*IDALsJacTimesVecFn)(realtype tt, N_Vector yy,
                                  N_Vector yp, N_Vector rr,
                                  N_Vector v, N_Vector Jv,
                                  realtype cj, void *user_data,
                                  N_Vector tmp1, N_Vector tmp2);
```

Purpose This function computes the product Jv of the DAE system Jacobian J (or an approximation to it) and a given vector `v`, where J is defined by Eq. (2.5).

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 (α 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,
                                    N_Vector yp, N_Vector rr,
                                    realtype cj, void *user_data);
```

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

Arguments
- `tt` is the current value of the independent variable.
- `yy` is the current value of the dependent variable vector, $y(t)$.

`yp` is the current value of $\dot{y}(t)$.

`rr` is the current value of the residual vector $F(t, y, \dot{y})$.

`cj` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.5)).

`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,
                                N_Vector yp, N_Vector rr,
                                N_Vector rvec, N_Vector zvec,
                                realtype cj, realtype delta,
                                void *user_data);
```

Purpose This function solves the preconditioning system $Pz = r$.

Arguments

`tt` is the current value of the independent variable.

`yy` is the current value of the dependent variable vector, $y(t)$.

`yp` is the current value of $\dot{y}(t)$.

`rr` is the current value of the residual vector $F(t, y, \dot{y})$.

`rvec` is the right-hand side vector r of the linear system to be solved.

`zvec` is the computed output vector.

`cj` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.5)).

`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,
                                N_Vector yp, N_Vector rr,
                                realtype cj, void *user_data);
```

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

Arguments
- `tt` is the current value of the independent variable.
- `yy` is the current value of the dependent variable vector, $y(t)$.
- `yp` is the current value of $\dot{y}(t)$.
- `rr` is the current value of the residual vector $F(t, y, \dot{y})$.
- `cj` is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.5)).
- `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.

With the default nonlinear solver (the native SUNDIALS Netwon method), 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. In the case of a user-supplied or external nonlinear solver, this is also true if the residual function is evaluated prior to calling the linear solver setup function (see §10.1.4 for more information).

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 [36] 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 `mudq` + `mldq` +2 evaluations of G_m, but only a matrix of bandwidth `mukeep` + `mlkeep` +1 is retained.

Neither pair of parameters need be the true half-bandwidths of the Jacobians of the local block of G, if smaller values provide a more efficient preconditioner. Such an efficiency gain may occur if the couplings in the DAE system outside a certain bandwidth are considerably weaker than those within the band. Reducing `mukeep` and `mlkeep` while keeping `mudq` and `mldq` at their true values, discards the elements outside the narrower band. Reducing both pairs has the additional effect of lumping the outer Jacobian elements into the computed elements within the band, and requires more caution and experimentation.

The solution of the complete linear system

$$Px = b \tag{4.4}$$

reduces to solving each of the equations

$$P_m x_m = b_m \tag{4.5}$$

and this is done by banded LU factorization of P_m followed by a banded backsolve.

Similar block-diagonal preconditioners could be considered with different treatment of the blocks P_m. For example, incomplete LU factorization or an iterative method could be used instead of banded LU factorization.

The IDABBDPRE module calls two user-provided functions to construct P: a required function `Gres` (of type `IDABBDLocalFn`) which approximates the residual function $G(t, y, \dot{y}) \approx F(t, y, \dot{y})$ and which is computed locally, and an optional function `Gcomm` (of type `IDABBDCommFn`) which performs all inter-process communication necessary to evaluate the approximate residual G. These are in addition to the user-supplied residual function `res`. Both functions take as input the same pointer `user_data` as passed by the user to `IDASetUserData` and passed to the user's function `res`. The user is responsible for providing space (presumably within `user_data`) for components of `yy` and `yp` that are communicated by `Gcomm` from the other processors, and that are then used by `Gres`, which should not do any communication.

`IDABBDLocalFn`

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

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

Arguments

`Nlocal`	is the local vector length.
`tt`	is the value of the independent variable.
`yy`	is the dependent variable.
`yp`	is the derivative of the dependent variable.
`gval`	is the output vector.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDABBDLocalFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes This function must assume that all inter-processor communication of data needed to calculate `gval` has already been done, and this data is accessible within `user_data`.

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

`IDABBDCommFn`

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

Purpose This `Gcomm` function performs all inter-processor communications necessary for the execution of the `Gres` function above, using the input vectors `yy` and `yp`.

Arguments

`Nlocal`	is the local vector length.
`tt`	is the value of the independent variable.
`yy`	is the dependent variable.
`yp`	is the derivative of the dependent variable.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

Return value An `IDABBDCommFn` function type should return 0 to indicate success, 1 for a recoverable error, or -1 for a non-recoverable error.

Notes The `Gcomm` function is expected to save communicated data in space defined within the structure `user_data`.

Each call to the `Gcomm` function is preceded by a call to the residual function `res` with the same (`tt`, `yy`, `yp`) arguments. Thus `Gcomm` can omit any communications done by `res` if relevant to the evaluation of `Gres`. If all necessary communication was done in `res`, then `Gcomm` = `NULL` can be passed in the call to `IDABBDPrecInit` (see below).

Besides the header files required for the integration of the DAE problem (see §4.3), to use the IDABBDPRE module, the main program must include the header file `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 IDABBDPRE 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.

F2003 Name `FIDABBDPrecInit`

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.

F2003 Name `FIDABBDPrecReInit`

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`.

F2003 Name `FIDABBDPrecGetWorkSpace`

`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.

F2003 Name `FIDABBDPrecGetNumGfnEvals`

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

Using IDA for Fortran Applications

A Fortran 2003 module (`fida_mod`) as well as a Fortran 77 style interface (FIDA) are provided to support the use of IDA, 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.

5.1 IDA Fortran 2003 Interface Module

The `fida_mod` Fortran module defines interfaces to most IDA C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. All interfaced functions are named after the corresponding C function, but with a leading 'F'. For example, the IDA function `IDACreate` is interfaced as `FIDACreate`. Thus, the steps to use IDA and the function calls in Fortran 2003 are identical (ignoring language differences) to those in C. The C functions with Fortran 2003 interfaces indicate this in their description in Chapter 4. The Fortran 2003 IDA interface module can be accessed by the `use` statement, i.e. `use fida_mod`, and linking to the library `libsundials_fida_mod.`*lib* in addition to `libsundials_ida.`*lib*.

The Fortran 2003 interface modules were generated with SWIG Fortran, a fork of SWIG [37]. Users who are interested in the SWIG code used in the generation process should contact the SUNDIALS *development team.*

5.1.1 SUNDIALS Fortran 2003 Interface Modules

All of the generic SUNDIALS modules provide Fortran 2003 interface modules. Many of the generic module implementations provide Fortran 2003 interfaces (a complete list of modules with Fortran 2003 interfaces is given in Table 5.1). A module can be accessed with the `use` statement, e.g. `use fnvector_openmp_mod`, and linking to the Fortran 2003 library in addition to the C library, e.g. `libsundials_fnvecpenmp_mod.`*lib* and `libsundials_nvecopenmp.`*lib*.

The Fortran 2003 interfaces leverage the `iso_c_binding` module and the `bind(C)` attribute to closely follow the SUNDIALS C API (ignoring language differences). The generic SUNDIALS structures, e.g. `N_Vector`, are interfaced as Fortran derived types, and function signatures are matched but with an `F` prepending the name, e.g. `FN_VConst` instead of `N_VConst`. Constants are named exactly as they are in the C API. Accordingly, using SUNDIALS via the Fortran 2003 interfaces looks just like using it in C. Some caveats stemming from the language differences are discussed in the section 5.1.3. A discussion on the topic of equivalent data types in C and Fortran 2003 is presented in section 5.1.2.

Further information on the Fortran 2003 interfaces specific to modules is given in the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL alongside the C documentation (chapters 7, 8, 9, and 10 respectively). For details on where the Fortran 2003 module (`.mod`) files and libraries are installed see Appendix A.

Table 5.1: Summary of Fortran 2003 interfaces for shared SUNDIALS modules.

Module	Fortran 2003 Module Name
NVECTOR	`fsundials_nvector_mod`
NVECTOR_SERIAL	`fnvector_serial_mod`
NVECTOR_PARALLEL	`fnvector_parallel_mod`
NVECTOR_OPENMP	`fnvector_openmp_mod`
NVECTOR_PTHREADS	`fnvector_pthreads_mod`
NVECTOR_PARHYP	Not interfaced
NVECTOR_PETSC	Not interfaced
NVECTOR_CUDA	Not interfaced
NVECTOR_RAJA	Not interfaced
NVECTOR_MANYVECTOR	`fnvector_manyvector_mod`
NVECTOR_MPIMANYVECTOR	`fnvector_mpimanyvector_mod`
NVECTOR_MPIPLUSX	`fnvector_mpiplusx_mod`
SUNMatrix	`fsundials_matrix_mod`
SUNMATRIX_BAND	`fsunmatrix_band_mod`
SUNMATRIX_DENSE	`fsunmatrix_dense_mod`
SUNMATRIX_SPARSE	`fsunmatrix_sparse_mod`
SUNLinearSolver	`fsundials_linearsolver_mod`
SUNLINSOL_BAND	`fsunlinsol_band_mod`
SUNLINSOL_DENSE	`fsunlinsol_dense_mod`
SUNLINSOL_LAPACKBAND	Not interfaced
SUNLINSOL_LAPACKDENSE	Not interfaced
SUNLINSOL_KLU	`fsunlinsol_klu_mod`
SUNLINSOL_SUPERLUMT	Not interfaced
SUNLINSOL_SUPERLUDIST	Not interfaced
SUNLINSOL_SPGMR	`fsunlinsol_spgmr_mod`
SUNLINSOL_SPFGMR	`fsunlinsol_spfgmr_mod`
SUNLINSOL_SPBCGS	`fsunlinsol_spbcgs_mod`
SUNLINSOL_SPTFQMR	`fsunlinsol_sptfqmr_mod`
SUNLINSOL_PCG	`fsunlinsol_pcg_mod`
SUNNonlinearSolver	`fsundials_nonlinearsolver_mod`
SUNNONLINSOL_NEWTON	`fsunnonlinsol_newton_mod`
SUNNONLINSOL_FIXEDPOINT	`fsunnonlinsol_fixedpoint_mod`

5.1.2 Data Types

Generally, the Fortran 2003 type that is equivalent to the C type is what one would expect. Primitive types map to the `iso_c_binding` type equivalent. SUNDIALS generic types map to a Fortran derived type. However, the handling of pointer types is not always clear as they can depend on the parameter direction. Table 5.2 presents a summary of the type equivalencies with the parameter direction in mind.

Currently, the Fortran 2003 interfaces are only compatible with SUNDIALS builds where the `realtype` is double precision and the `sunindextype` size is 64-bits.

5.1.3 Notable Fortran/C usage differences

While the Fortran 2003 interface to SUNDIALS closely follows the C API, some differences are inevitable due to the differences between Fortran and C. In this section, we note the most critical differences. Additionally, section 5.1.2 discusses equivalencies of data types in the two languages.

Table 5.2: C/Fortran 2003 Equivalent Types

C type	Parameter Direction	Fortran 2003 type
double	in, inout, out, return	real(c_double)
int	in, inout, out, return	integer(c_int)
long	in, inout, out, return	integer(c_long)
booleantype	in, inout, out, return	integer(c_int)
realtype	in, inout, out, return	real(c_double)
sunindextype	in, inout, out, return	integer(c_long)
double*	in, inout, out	real(c_double), dimension(*)
double*	return	real(c_double), pointer, dimension(:)
int*	in, inout, out	integer(c_int), dimension(*)
int*	return	integer(c_int), pointer, dimension(:)
long*	in, inout, out	integer(c_long), dimension(*)
long*	return	integer(c_long), pointer, dimension(:)
realtype*	in, inout, out	real(c_double), dimension(*)
realtype*	return	real(c_double), pointer, dimension(:)
sunindextype*	in, inout, out	integer(c_long), dimension(*)
sunindextype*	return	integer(c_long), pointer, dimension(:)
realtype[]	in, inout, out	real(c_double), dimension(*)
sunindextype[]	in, inout, out	integer(c_long), dimension(*)
N_Vector	in, inout, out	type(N_Vector)
N_Vector	return	type(N_Vector), pointer
SUNMatrix	in, inout, out	type(SUNMatrix)
SUNMatrix	return	type(SUNMatrix), pointer
SUNLinearSolver	in, inout, out	type(SUNLinearSolver)
SUNLinearSolver	return	type(SUNLinearSolver), pointer
SUNNonlinearSolver	in, inout, out	type(SUNNonlinearSolver)
SUNNonlinearSolver	return	type(SUNNonlinearSolver), pointer
FILE*	in, inout, out, return	type(c_ptr)
void*	in, inout, out, return	type(c_ptr)
T**	in, inout, out, return	type(c_ptr)
T***	in, inout, out, return	type(c_ptr)
T****	in, inout, out, return	type(c_ptr)

5.1.3.1 Creating generic SUNDIALS objects

In the C API a generic SUNDIALS object, such as an `N_Vector`, is actually a pointer to an underlying C struct. However, in the Fortran 2003 interface, the derived type is bound to the C struct, not the pointer to the struct. E.g., `type(N_Vector)` is bound to the C struct `_generic_N_Vector` not the `N_Vector` type. The consequence of this is that creating and declaring SUNDIALS objects in Fortran is nuanced. This is illustrated in the code snippets below:

C *code*:

```
N_Vector x;
x = N_VNew_Serial(N);
```

Fortran code:

```
type(N_Vector), pointer :: x
x => FN_VNew_Serial(N)
```

Note that in the Fortran declaration, the vector is a `type(N_Vector), pointer`, and that the pointer assignment operator is then used.

5.1.3.2 Arrays and pointers

Unlike in the C API, in the Fortran 2003 interface, arrays and pointers are treated differently when they are return values versus arguments to a function. Additionally, pointers which are meant to be out parameters, not arrays, in the C API must still be declared as a rank-1 array in Fortran. The reason for this is partially due to the Fortran 2003 standard for C bindings, and partially due to the tool used to generate the interfaces. Regardless, the code snippets below illustrate the differences.

C *code*:

```
N_Vector x
realtype* xdata;
long int leniw, lenrw;

x = N_VNew_Serial(N);

/* capturing a returned array/pointer */
xdata = N_VGetArrayPointer(x)

/* passing array/pointer to a function */
N_VSetArrayPointer(xdata, x)

/* pointers that are out-parameters */
N_VSpace(x, &leniw, &lenrw);
```

Fortran code:

```
type(N_Vector), pointer :: x
real(c_double), pointer :: xdataptr(:)
real(c_double)          :: xdata(N)
integer(c_long)         :: leniw(1), lenrw(1)

x => FN_VNew_Serial(x)

! capturing a returned array/pointer
xdataptr => FN_VGetArrayPointer(x)

! passing array/pointer to a function
call FN_VSetArrayPointer(xdata, x)

! pointers that are out-parameters
call FN_VSpace(x, leniw, lenrw)
```

5.1.3.3 Passing procedure pointers and user data

Since functions/subroutines passed to SUNDIALS will be called from within C code, the Fortran procedure must have the attribute `bind(C)`. Additionally, when providing them as arguments to a Fortran 2003 interface routine, it is required to convert a procedure's Fortran address to C with the Fortran intrinsic `c_funloc`.

Typically when passing user data to a SUNDIALS function, a user may simply cast some custom data structure as a `void*`. When using the Fortran 2003 interfaces, the same thing can be achieved. Note, the custom data structure *does not* have to be `bind(C)` since it is never accessed on the C side.

C *code*:

```
MyUserData* udata;
```

```
void *cvode_mem;

ierr = CVodeSetUserData(cvode_mem, udata);
```

Fortran code:

```
type(MyUserData) :: udata
type(c_ptr)      :: cvode_mem

ierr = FCVodeSetUserData(cvode_mem, c_loc(udata))
```

On the other hand, Fortran users may instead choose to store problem-specific data, e.g. problem parameters, within modules, and thus do not need the SUNDIALS-provided `user_data` pointers to pass such data back to user-supplied functions. These users should supply the `c_null_ptr` input for `user_data` arguments to the relevant SUNDIALS functions.

5.1.3.4 Passing NULL to optional parameters

In the SUNDIALS C API some functions have optional parameters that a caller can pass `NULL` to. If the optional parameter is of a type that is equivalent to a Fortran `type(c_ptr)` (see section 5.1.2), then a Fortran user can pass the intrinsic `c_null_ptr`. However, if the optional parameter is of a type that is not equivalent to `type(c_ptr)`, then a caller must provide a Fortran pointer that is dissociated. This is demonstrated in the code example below.

C *code*:

```
SUNLinearSolver LS;
N_Vector x, b;

! SUNLinSolSolve expects a SUNMatrix or NULL
! as the second parameter.
ierr = SUNLinSolSolve(LS, NULL, x, b);
```

Fortran code:

```
type(SUNLinearSolver), pointer :: LS
type(SUNMatrix), pointer :: A
type(N_Vector), pointer :: x, b

A => null()

! SUNLinSolSolve expects a type(SUNMatrix), pointer
! as the second parameter. Therefore, we cannot
! pass a c_null_ptr, rather we pass a disassociated A.
ierr = FSUNLinSolSolve(LS, A, x, b)
```

5.1.3.5 Working with `N_Vector` arrays

Arrays of `N_Vector` objects are interfaced to Fortran 2003 as opaque `type(c_ptr)`. As such, it is not possible to directly index an array of `N_Vector` objects returned by the `N_Vector` "VectorArray" operations, or packages with sensitivity capablities. Instead, SUNDIALS provides a utility function `FN_VGetVecAtIndexVectorArray` that can be called for accessing a vector in a vector array. The example below demonstrates this:

C *code*:

```
N_Vector x;
N_Vector* vecs;

vecs = N_VCloneVectorArray(count, x);
for (int i=0; i < count; ++i)
  N_VConst(vecs[i]);
```

Fortran code:

```
type(N_Vector), pointer :: x, xi
type(c_ptr)             :: vecs

vecs = FN_VCloneVectorArray(count, x)
do index, count
  xi => FN_VGetVecAtIndexVectorArray(vecs, index)
  call FN_VConst(xi)
enddo
```

SUNDIALS also provides the functions `FN_VSetVecAtIndexVectorArray` and `FN_VNewVectorArray` for working with `N_Vector` arrays. These functions are particularly useful for users of the Fortran interface to the NVECTOR_MANYVECTOR or NVECTOR_MPIMANYVECTOR when creating the subvector array. Both of these functions along with `FN_VGetVecAtIndexVectorArray` are further described in Chapter 7.1.6.

5.1.3.6 Providing file pointers

Expert SUNDIALS users may notice that there are a few advanced functions in the SUNDIALS C API that take a `FILE *` argument. Since there is no portable way to convert between a Fortran file descriptor and a C file pointer, SUNDIALS provides two utility functions for creating a `FILE *` and destroying it. These functions are defined in the module `fsundials_futils_mod`.

`FSUNDIALSFileOpen`

Call `fp = FSUNDIALSFileOpen(filename, mode)`

Description The function allocates a `FILE *` by calling the C function `fopen`.

Arguments
- `filename` (`character(kind=C_CHAR, len=*)`) - the path to the file to open
- `mode` (`character(kind=C_CHAR, len=*)`) - the mode string given to `fopen` It should begin with one of the following characters:
  - "r" - open text file for reading
  - "r+" - open text file for reading and writing
  - "w" - truncate text file to zero length or create it for writing
  - "w+" - open text file for reading or writing, create it if it does not exist
  - "a" - open for appending, see documentation of "fopen" for your system/compiler
  - "a+" - open for reading and appending, see documentation for "fopen" for your system/compiler

Return value This returns a `type(C_PTR)` which is a `FILE*` in C. If it is `NULL`, then there was an error opening the file.

FSUNDIALSFileClose	
Call	`call FSUNDIALSFileClose(fp)`
Description	The function deallocates a `FILE*` by calling the C function `fclose`.
Arguments	`fp` (`type(C_PTR)`) - the file pointer (type `FILE*` in C)
Return value	None

5.1.4 Important notes on portability

The SUNDIALS Fortran 2003 interface *should* be compatible with any compiler supporting the Fortran 2003 ISO standard. However, it has only been tested and confirmed to be working with GNU Fortran 4.9+ and Intel Fortran 18.0.1+.

Upon compilation of SUNDIALS, Fortran module (`.mod`) files are generated for each Fortran 2003 interface. These files are highly compiler specific, and thus it is almost always necessary to compile a consuming application with the same compiler used to generate the modules.

5.2 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.

5.3 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).

5.4 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

5.4.1 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.

5.4.2 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 7.

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 8. 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 SUNDIALS, 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 9. 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 9.

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 5.4.

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. $\sqrt{\sum(\rho_i * \texttt{EWT}[i])^2} <$ 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 5.4).

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 5.3), 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 5.4 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 5.3: 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.	$\text{uround}^{2/3}$

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 5.4: 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	HO_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.

5.5.1 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$= 1, \ldots,$ 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.

5.5.2 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 §5.4.1, 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 §5.4.2 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 5.4. 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 §5.4.2.

Chapter 6

IDA Features for GPU Accelerated Computing

This chapter is concerned with using GPU-acceleration and IDA for the solution of DAEs.

6.1 SUNDIALS GPU Programming Model

In this section, we introduce the SUNDIALS GPU programming model and highlight SUNDIALS GPU features. The model leverages the fact that all of the SUNDIALS packages interact with simulation data either through the shared vector, matrix, and solver APIs (see §7, §8, §9, and §10) or through user-supplied callback functions. Thus, under the model, the overall structure of the user's calling program, and the way users interact with the SUNDIALS packages is similar to using SUNDIALS in CPU-only environments.

Within the SUNDIALS GPU programming model, all control logic executes on the CPU, and all simulation data resides wherever the vector or matrix object dictates as long as SUNDIALS is in control of the program. That is, SUNDIALS will not migrate data (explicitly) from one memory space to another. Except in the most advanced use cases, it is safe to assume that data is kept resident in the GPU-device memory space. The consequence of this is that, when control is passed from the user's calling program to SUNDIALS, simulation data in vector or matrix objects must be up-to-date in the device memory space. Similarly, when control is passed from SUNDIALS to the user's calling program, the user should assume that any simulation data in vector and matrix objects are up-to-date in the device memory space. To put it succinctly, *it is the responsibility of the user's calling program to manage data coherency between the CPU and GPU-device memory spaces* unless unified virtual memory (UVM), also known as managed memory, is being utilized. Typically, the GPU-enabled SUNDIALS modules provide functions to copy data from the host to the device and vice-versa as well as support for unmanaged memory or UVM. In practical terms, the way SUNDIALS handles distinct host and device memory spaces means that *users need to ensure that the user-supplied functions, e.g. the right-hand side function, only operate on simulation data in the device memory space* otherwise extra memory transfers will be required and performance will be poor. The exception to this rule is if some form of hybrid data partitioning (achievable with the NVECTOR_MANYVECTOR §7.15) is utilized.

SUNDIALS provides many native shared features and modules that are GPU-enabled. Currently, these are primarily limited to the NVIDIA CUDA platform [5], although support for more GPU computing platforms such as AMD ROCm/HIP [1] and Intel oneAPI [2], is an area of active development. Table 6.1 summarizes the shared SUNDIALS modules that are GPU-enabled, what GPU programming environments they support, and what class of memory they support (unmanaged or UVM). Users may also supply their own GPU-enabled `N_Vector`, `SUNMatrix`, `SUNLinearSolver`, or `SUNNonlinearSolver` implementation, and the capabilties will be leveraged since SUNDIALS operates on data through these APIs.

In addition, SUNDIALS provides the `SUNMemoryHelper` API §11.1 to support applications which

implement their own memory management or memory pooling.

Table 6.1: List of SUNDIALS GPU Enabled Modules. Note that support for ROCm/HIP and oneAPI are currently untested, and implicit UVM (i.e. `malloc` returning UVM) is not accounted for. A The † symbol indicates that the module inherits support from the NVECTOR module used.

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged memory	UVM
NVECTOR_CUDA (§7.9)	✓			✓	✓
NVECTOR_RAJA (§7.11)	✓			✓	✓
NVECTOR_OPENMPDEV (§7.13)	✓	✓	✓	✓	
SUNMATRIX_CUSPARSE (§8.7)	✓			✓	✓
SUNLINSOL_CUSOLVERSP_BATCHQR (§9.12)	✓			✓	✓
SUNLINSOL_SPGMR (§9.14)	†	†	†	†	†
SUNLINSOL_SPFGMR (§9.15)	†	†	†	†	†
SUNLINSOL_SPTFQMR (§9.17)	†	†	†	†	†
SUNLINSOL_SPBCGS (§9.16)	†	†	†	†	†
SUNLINSOL_PCG (§9.18)	†	†	†	†	†
SUNNONLINSOL_NEWTON (§10.3)	†	†	†	†	†
SUNNONLINSOL_FIXEDPOINT (§??)	†	†	†	†	†

6.2 Steps for Using GPU Accelerated SUNDIALS

For any SUNDIALS package, the generalized steps a user needs to take to use GPU accelerated SUNDIALS are:

1. Utilize a GPU-enabled NVECTOR implementation. Initial data can be loaded on the host, but must be in the device memory space prior to handing control to SUNDIALS.
2. Utilize a GPU-enabled SUNLINSOL linear solver (if necessary).
3. Utilize a GPU-enabled SUNMATRIX implementation (if using a matrix-based linear solver).
4. Utilize a GPU-enabled SUNNONLINSOL nonlinear solver (if necessary).
5. Write user-supplied functions so that they use data only in the device memory space (again, unless an atypical data partitioning is used). A few examples of these functions are the right-hand side evaluation function, the Jacobian evalution function, or the preconditioner evaluation function. In the context of CUDA and the right-hand side function, one way a user might ensure data is accessed on the device is, for example, calling a CUDA kernel, which does all of the computation, from a CPU function which simply extracts the underlying device data array from the NVECTOR object that is passed from SUNDIALS to the user-supplied function.

Users should refer to Table 6.1 for a list of GPU-enabled native SUNDIALS modules.

Chapter 7

Description of the NVECTOR module

The SUNDIALS solvers are written in a data-independent manner. They all operate on generic vectors (of type `N_Vector`) through a set of operations defined by the particular NVECTOR implementation. Users can provide their own specific implementation of the NVECTOR module, or use one of the implementations provided with SUNDIALS. The generic NVECTOR is described below and the implementations provided with SUNDIALS are described in the following sections.

7.1 The NVECTOR API

The generic NVECTOR API can be broken down into groups of functions: the core vector operations, the fused vector operations, the vector array operations, the local reduction operations, the exchange operations, and finally some utility functions. All but the last group are defined by a particular NVECTOR implementation. The utility functions are defined by the generic NVECTOR itself.

7.1.1 NVECTOR core functions

`N_VGetVectorID`

Call `id = N_VGetVectorID(w);`

Description 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.

Arguments `w` (`N_Vector`) a NVECTOR object

Return value This function returns an `N_Vector_ID`. Possible values are given in Table 7.1.

F2003 Name `FN_VGetVectorID`

`N_VClone`

Call `v = N_VClone(w);`

Description 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.

Arguments `w` (`N_Vector`) a NVECTOR object

Return value This function returns an `N_Vector` object. If an error occurs, then this routine will return `NULL`.

F2003 Name `FN_VClone`

`N_VCloneEmpty`

Call `v = N_VCloneEmpty(w);`

Description 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.

Arguments `w` (`N_Vector`) a NVECTOR object

Return value This function returns an `N_Vector` object. If an error occurs, then this routine will return `NULL`.

F2003 Name `FN_VCloneEmpty`

`N_VDestroy`

Call `N_VDestroy(v);`

Description Destroys the `N_Vector` `v` and frees memory allocated for its internal data.

Arguments `v` (`N_Vector`) a NVECTOR object to destroy

Return value None

F2003 Name `FN_VDestroy`

`N_VSpace`

Call `N_VSpace(v, &lrw, &liw);`

Description 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.

Arguments `v` (`N_Vector`) a NVECTOR object

`lrw` (`sunindextype*`) out parameter containing the number of realtype words

`liw` (`sunindextype*`) out parameter containing the number of integer words

Return value None

F2003 Name `FN_VSpace`

F2003 Call
```
integer(c_long) ::  lrw(1), liw(1)
call FN_VSpace_Serial(v, lrw, liw)
```

`N_VGetArrayPointer`

Call `vdata = N_VGetArrayPointer(v);`

Description 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` and is accessible from the CPU.

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.

Arguments `v` (`N_Vector`) a NVECTOR object

Return value `realtype*`

F2003 Name `FN_VGetArrayPointer`

`N_VGetDeviceArrayPointer`

Call `vdata = N_VGetDeviceArrayPointer(v);`

Description Returns a device 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` and is accessible from the device (e.g., GPU).

This operation is *optional* except when using the GPU-enabled direct linear solvers.

Arguments `v` (`N_Vector`) a NVECTOR object

Return value `realtype*`

Notes Currently, only the GPU-enabled SUNDIALS vectors provide this operation. All other SUNDIALS vectors will return `NULL`.

F2003 Name `FN_VGetDeviceArrayPointer`

`N_VSetArrayPointer`

Call `N_VSetArrayPointer(vdata, v);`

Description Overwrites the pointer to the data in an `N_Vector` with a given `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.

Arguments `v` (`N_Vector`) a NVECTOR object

Return value None

F2003 Name `FN_VSetArrayPointer`

`N_VGetCommunicator`

Call `N_VGetCommunicator(v);`

Description Returns a pointer to the `MPI_Comm` object associated with the vector (if applicable). For MPI-unaware vector implementations, this should return `NULL`.

Arguments `v` (`N_Vector`) a NVECTOR object

Return value A `void *` pointer to the `MPI_Comm` object if the vector is MPI-aware, otherwise `NULL`.

F2003 Name `FN_VGetCommunicator`

`N_VGetLength`

Call `N_VGetLength(v);`

Description 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.

Arguments `v` (`N_Vector`) a NVECTOR object

Return value `sunindextype`

F2003 Name `FN_VGetLength`

`N_VLinearSum`

Call `N_VLinearSum(a, x, b, y, z);`

Description Performs the operation $z = ax + by$, where a and b are `realtype` scalars and x and y are of type `N_Vector`: $z_i = ax_i + by_i$, $i = 0, \ldots, n-1$.

Arguments `a` (`realtype`) constant that scales `x`
`x` (`N_Vector`) a NVECTOR object
`b` (`realtype`) constant that scales `y`
`y` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value The output vector `z` can be the same as either of the input vectors (`x` or `y`).

F2003 Name `FN_VLinearSum`

`N_VConst`

Call `N_VConst(c, z);`

Description Sets all components of the `N_Vector z` to `realtype c`: $z_i = c$, $i = 0, \ldots, n-1$.

Arguments `c` (`realtype`) constant to set all components of `z` to
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VConst`

`N_VProd`

Call `N_VProd(x, y, z);`

Description Sets the `N_Vector z` to be the component-wise product of the `N_Vector` inputs `x` and `y`: $z_i = x_i y_i$, $i = 0, \ldots, n-1$.

Arguments `x` (`N_Vector`) a NVECTOR object
`y` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VProd`

`N_VDiv`

Call `N_VDiv(x, y, z);`

Description 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.

Arguments `x` (`N_Vector`) a NVECTOR object
`y` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VDiv`

`N_VScale`

Call `N_VScale(c, x, z);`

Description Scales the `N_Vector` `x` by the `realtype` scalar `c` and returns the result in `z`: $z_i = cx_i, i = 0, \ldots, n-1$.

Arguments `c` (`realtype`) constant that scales the vector `x`
`x` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VScale`

`N_VAbs`

Call `N_VAbs(x, z);`

Description Sets the components of the `N_Vector` `z` to be the absolute values of the components of the `N_Vector` `x`: $z_i = |x_i|$, $i = 0, \ldots, n-1$.

Arguments `x` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VAbs`

`N_VInv`

Call `N_VInv(x, z);`

Description 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.

Arguments `x` (`N_Vector`) a NVECTOR object to
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VInv`

`N_VAddConst`

Call `N_VAddConst(x, b, z);`

Description Adds the `realtype` scalar `b` to all components of `x` and returns the result in the `N_Vector` `z`: $z_i = x_i + b$, $i = 0, \ldots, n-1$.

Arguments `x` (`N_Vector`) a NVECTOR object
`b` (`realtype`) constant added to all components of `x`
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VAddConst`

`N_VDotProd`

Call `d = N_VDotProd(x, y);`

Description Returns the value of the ordinary dot product of `x` and `y`: $d = \sum_{i=0}^{n-1} x_i y_i$.

Arguments `x` (`N_Vector`) a NVECTOR object with `y`
`y` (`N_Vector`) a NVECTOR object with `x`

Return value `realtype`

F2003 Name `FN_VDotProd`

`N_VMaxNorm`

Call `m = N_VMaxNorm(x);`

Description Returns the maximum norm of the `N_Vector x`: $m = \max_i |x_i|$.

Arguments `x` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VMaxNorm`

`N_VWrmsNorm`

Call `m = N_VWrmsNorm(x, w)`

Description Returns the weighted root-mean-square norm of the `N_Vector x` with `realtype` weight vector `w`: $m = \sqrt{\left(\sum_{i=0}^{n-1}(x_i w_i)^2\right)/n}$.

Arguments `x` (`N_Vector`) a NVECTOR object
`w` (`N_Vector`) a NVECTOR object containing weights

Return value `realtype`

F2003 Name `FN_VWrmsNorm`

`N_VWrmsNormMask`

Call `m = N_VWrmsNormMask(x, w, id);`

Description 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 $H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$

Arguments `x` (`N_Vector`) a NVECTOR object
`w` (`N_Vector`) a NVECTOR object containing weights
`id` (`N_Vector`) mask vector

Return value `realtype`

F2003 Name `FN_VWrmsNormMask`

`N_VMin`

Call `m = N_VMin(x);`

Description Returns the smallest element of the `N_Vector x`: $m = \min_i x_i$.

Arguments `x` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VMin`

`N_VWL2Norm`

Call `m = N_VWL2Norm(x, w);`

Description Returns the weighted Euclidean ℓ_2 norm of the `N_Vector` `x` with `realtype` weight vector `w`: $m = \sqrt{\sum_{i=0}^{n-1}(x_i w_i)^2}$.

Arguments `x` (`N_Vector`) a NVECTOR object
`w` (`N_Vector`) a NVECTOR object containing weights

Return value `realtype`

F2003 Name `FN_VWL2Norm`

`N_VL1Norm`

Call `m = N_VL1Norm(x);`

Description Returns the ℓ_1 norm of the `N_Vector` `x`: $m = \sum_{i=0}^{n-1} |x_i|$.

Arguments `x` (`N_Vector`) a NVECTOR object to obtain the norm of

Return value `realtype`

F2003 Name `FN_VL1Norm`

`N_VCompare`

Call `N_VCompare(c, x, z);`

Description 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.

Arguments `c` (`realtype`) constant that each component of `x` is compared to
`x` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) a NVECTOR object containing the result

Return value None

F2003 Name `FN_VCompare`

`N_VInvTest`

Call `t = N_VInvTest(x, z);`

Description 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: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$.

Arguments `x` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) an output NVECTOR object

Return value Returns a `booleantype` with value `SUNTRUE` if all components of `x` are nonzero (successful inversion) and returns `SUNFALSE` otherwise.

F2003 Name `FN_VInvTest`

`N_VConstrMask`

Call `t = N_VConstrMask(c, x, m);`

Description 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.

Arguments `c` (`realtype`) scalar constraint value
`x` (`N_Vector`) a NVECTOR object
`m` (`N_Vector`) output mask vector

Return value Returns a `booleantype` with value `SUNFALSE` if any element failed the constraint test, and `SUNTRUE` if all passed.

F2003 Name `FN_VConstrMask`

`N_VMinQuotient`

Call `minq = N_VMinQuotient(num, denom);`

Description This routine returns the minimum of the quotients obtained by term-wise dividing $\texttt{num}_i$ by $\texttt{denom}_i$. A zero element in `denom` will be skipped. If no such quotients are found, then the large value `BIG_REAL` (defined in the header file `sundials_types.h`) is returned.

Arguments `num` (`N_Vector`) a NVECTOR object used as the numerator
`denom` (`N_Vector`) a NVECTOR object used as the denominator

Return value `realtype`

F2003 Name `FN_VMinQuotient`

7.1.2 NVECTOR fused functions

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.

`N_VLinearCombination`

Call `ier = N_VLinearCombination(nv, c, X, z);`

Description 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, X is an array of n_v vectors, and z is the output vector.

Arguments `nv` (`int`) the number of vectors in the linear combination
`c` (`realtype*`) an array of n_v scalars used to scale the corresponding vector in `X`
`X` (`N_Vector*`) an array of n_v NVECTOR objects to be scaled and combined
`z` (`N_Vector`) a NVECTOR object containing the result

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

Notes If the output vector z is one of the vectors in X, then it *must* be the first vector in the vector array.

F2003 Name `FN_VLinearCombination`

F2003 Call
```
real(c_double) ::  c(nv)
type(c_ptr), target ::  X(nv)
type(N_Vector), pointer ::  z
ierr = FN_VLinearCombination(nv, c, X, z)
```

`N_VScaleAddMulti`

Call `ier = N_VScaleAddMulti(nv, c, x, Y, Z);`

Description 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, x is the vector to be scaled and added to each vector in the vector array of n_v vectors Y, and Z is a vector array of n_v output vectors.

Arguments
- `nv` (`int`) the number of scalars and vectors in `c`, `Y`, and `Z`
- `c` (`realtype*`) an array of n_v scalars
- `x` (`N_Vector`) a NVECTOR object to be scaled and added to each vector in `Y`
- `Y` (`N_Vector*`) an array of n_v NVECTOR objects where each vector j will have the vector `x` scaled by `c_j` added to it
- `Z` (`N_Vector`) an output array of n_v NVECTOR objects

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VScaleAddMulti`

F2003 Call
```
real(c_double) ::  c(nv)
type(c_ptr), target ::  Y(nv), Z(nv)
type(N_Vector), pointer ::  x
ierr = FN_VScaleAddMulti(nv, c, x, Y, Z)
```

`N_VDotProdMulti`

Call `ier = N_VDotProdMulti(nv, x, Y, d);`

Description 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 is an array of n_v scalars containing the dot products of the vector x with each of the n_v vectors in the vector array Y.

Arguments
- `nv` (`int`) the number of vectors in `Y`
- `x` (`N_Vector`) a NVECTOR object to be used in a dot product with each of the vectors in `Y`
- `Y` (`N_Vector*`) an array of n_v NVECTOR objects to use in a dot product with `x`
- `d` (`realtype*`) an output array of n_v dot products

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VDotProdMulti`

F2003 Call
```
real(c_double) ::  d(nv)
type(c_ptr), target ::  Y(nv)
type(N_Vector), pointer ::  x
ierr = FN_VDotProdMulti(nv, x, Y, d)
```

7.1.3 NVECTOR vector array functions

`N_VLinearSumVectorArray`

Call `ier = N_VLinearSumVectorArray(nv, a, X, b, Y, Z);`

Description 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 scalars and X, Y, and Z are arrays of n_v vectors.

Arguments
- `nv` (`int`) the number of vectors in the vector arrays
- `a` (`realtype`) constant to scale each vector in `X` by
- `X` (`N_Vector*`) an array of n_v NVECTOR objects
- `Y` (`N_Vector*`) an array of n_v NVECTOR objects
- `Z` (`N_Vector*`) an output array of n_v NVECTOR objects

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VLinearSumVectorArray`

`N_VScaleVectorArray`

Call `ier = N_VScaleVectorArray(nv, c, X, Z);`

Description 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 and X and Z are arrays of n_v vectors.

Arguments
- `nv` (`int`) the number of vectors in the vector arrays
- `c` (`realtype`) constant to scale each vector in `X` by
- `X` (`N_Vector*`) an array of n_v NVECTOR objects
- `Z` (`N_Vector*`) an output array of n_v NVECTOR objects

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VScaleVectorArray`

`N_VConstVectorArray`

Call `ier = N_VConstVectorArray(nv, c, X);`

Description 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 scalar and X is an array of n_v vectors.

Arguments
- `nv` (`int`) the number of vectors in `X`
- `c` (`realtype`) constant to set every element in every vector of `X` to
- `X` (`N_Vector*`) an array of n_v NVECTOR objects

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VConstVectorArray`

`N_VWrmsNormVectorArray`

Call `ier = N_VWrmsNormVectorArray(nv, X, W, m);`

Description This routine computes the weighted root mean square norm of n_v vectors with n elements:

$$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i})^2 \right)^{1/2}, \quad j = 0, \ldots, n_v - 1,$$

where m contains the n_v norms of the vectors in the vector array X with corresponding weight vectors W.

Arguments
- `nv` (`int`) the number of vectors in the vector arrays
- `X` (`N_Vector*`) an array of n_v NVECTOR objects
- `W` (`N_Vector*`) an array of n_v NVECTOR objects
- `m` (`realtype*`) an output array of n_v norms

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VWrmsNormVectorArray`

`N_VWrmsNormMaskVectorArray`

Call `ier = N_VWrmsNormMaskVectorArray(nv, X, W, id, m);`

Description This routine computes the masked weighted root mean square norm of n_v vectors with n elements:

$$m_j = \left(\frac{1}{n} \sum_{i=0}^{n-1} (x_{j,i} w_{j,i} H(id_i))^2 \right)^{1/2}, \quad j = 0, \ldots, n_v - 1,$$

$H(id_i) = 1$ for $id_i > 0$ and is zero otherwise, m contains the n_v norms of the vectors in the vector array X with corresponding weight vectors W and mask vector id.

Arguments
- `nv` (`int`) the number of vectors in the vector arrays
- `X` (`N_Vector*`) an array of n_v NVECTOR objects
- `W` (`N_Vector*`) an array of n_v NVECTOR objects
- `id` (`N_Vector`) the mask vector
- `m` (`realtype*`) an output array of n_v norms

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VWrmsNormMaskVectorArray`

`N_VScaleAddMultiVectorArray`

Call `ier = N_VScaleAddMultiVectorArray(nv, ns, c, X, YY, ZZ);`

Description This routine scales and adds a vector in a vector array of n_v vectors to the corresponding vector in n_s vector arrays:

$$z_{k,j,i} = c_k x_{j,i} + y_{k,j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, nv-1, \quad k = 0, \ldots, ns-1$$

where c is an array of n_s scalars, X is a vector array of n_v vectors to be scaled and added to the corresponding vector in each of the n_s vector arrays in the array of vector arrays YY and stored in the output array of vector arrays ZZ.

Arguments
- `nv` (`int`) the number of vectors in the vector arrays
- `ns` (`int`) the number of scalars in `c` and vector arrays in `YY` and `ZZ`
- `c` (`realtype*`) an array of n_s scalars

`X` (`N_Vector*`) an array of n_v NVECTOR objects

`YY` (`N_Vector**`) an array of n_s NVECTOR arrays

`ZZ` (`N_Vector**`) an output array of n_s NVECTOR arrays

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

`N_VLinearCombinationVectorArray`

Call `ier = N_VLinearCombinationVectorArray(nv, ns, c, XX, Z);`

Description 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.

Arguments `nv` (`int`) the number of vectors in the vector arrays

`ns` (`int`) the number of scalars in `c` and vector arrays in `YY` and `ZZ`

`c` (`realtype*`) an array of n_s scalars

`XX` (`N_Vector**`) an array of n_s NVECTOR arrays

`Z` (`N_Vector*`) an output array NVECTOR objects

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

7.1.4 NVECTOR local reduction functions

Local reduction operations are intended to reduce parallel communication on distributed memory systems, particularly when NVECTOR objects are combined together within a NVECTOR_MPIMANYVECTOR object (see Section 7.16). If a particular NVECTOR implementation defines a local reduction operation as `NULL`, the NVECTOR_MPIMANYVECTOR 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.

`N_VDotProdLocal`

Call `d = N_VDotProdLocal(x, y);`

Description 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).

Arguments `x` (`N_Vector`) a NVECTOR object

`y` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VDotProdLocal`

`N_VMaxNormLocal`

Call `m = N_VMaxNormLocal(x);`

Description 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).

Arguments `x` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VMaxNormLocal`

`N_VMinLocal`

Call `m = N_VMinLocal(x);`

Description 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).

Arguments `x` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VMinLocal`

`N_VL1NormLocal`

Call `n = N_VL1NormLocal(x);`

Description 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).

Arguments `x` (`N_Vector`) a NVECTOR object

Return value `realtype`

F2003 Name `FN_VL1NormLocal`

`N_VWSqrSumLocal`

Call `s = N_VWSqrSumLocal(x,w);`

Description 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).

Arguments `x` (`N_Vector`) a NVECTOR object
`w` (`N_Vector`) a NVECTOR object containing weights

Return value `realtype`

F2003 Name `FN_VWSqrSumLocal`

`N_VWSqrSumMaskLocal`

Call `s = N_VWSqrSumMaskLocal(x,w,id);`

Description 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`:

$$m = \sum_{i=0}^{n_{local}-1} (x_i w_i H(id_i))^2, \quad \text{where} \quad H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$$

and n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).

Arguments `x` (`N_Vector`) a NVECTOR object
`w` (`N_Vector`) a NVECTOR object containing weights
`id` (`N_Vector`) a NVECTOR object used as a mask

Return value `realtype`

F2003 Name `FN_VWSqrSumMaskLocal`

`N_VInvTestLocal`

Call `t = N_VInvTestLocal(x, z);`

Description 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:

$$z_i = 1.0/x_i,\ i = 0, \ldots, n_{local} - 1,$$

where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications).

Arguments `x` (`N_Vector`) a NVECTOR object
`z` (`N_Vector`) an output NVECTOR object

Return value Returns a `booleantype` with the value `SUNTRUE` if all task-local components of `x` are nonzero (successful inversion) and with the value `SUNFALSE` otherwise.

F2003 Name `FN_VInvTestLocal`

`N_VConstrMaskLocal`

Call `t = N_VConstrMaskLocal(c,x,m);`

Description 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. It 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.

Arguments `c` (`realtype`) scalar constraint value
`x` (`N_Vector`) a NVECTOR object
`m` (`N_Vector`) output mask vector

Return value Returns a `booleantype` with the value `SUNFALSE` if any task-local element failed the constraint test and the value `SUNTRUE` if all passed.

F2003 Name `FN_VConstrMaskLocal`

`N_VMinQuotientLocal`

Call `minq = N_VMinQuotientLocal(num,denom);`

Description This routine returns the minimum of the quotients obtained by term-wise dividing $\texttt{num}_i$ by $\texttt{denom}_i$, 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.

Arguments `num` (`N_Vector`) a NVECTOR object used as the numerator
`denom` (`N_Vector`) a NVECTOR object used as the denominator

Return value `realtype`

F2003 Name `FN_VMinQuotientLocal`

7.1.5 NVECTOR exchange operations

The following vector exchange operations are also *optional* and are intended only for use when interfacing with the XBraid library for parallel-in-time integration. In that setting these operations are required but are otherwise unused by SUNDIALS packages and may be set to `NULL`. For each operation, we give the function signature, a description of the expected behavior, and an example of the function usage.

`N_VBufSize`

Call `flag = N_VBufSize(N_Vector x, sunindextype *size);`

Description This routine returns the buffer size need to exchange in the data in the vector `x` between computational nodes.

Arguments `x` (`N_Vector`) a NVECTOR object
`size` (`sunindextype*`) the size of the message buffer

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VBufSize`

`N_VBufPack`

Call `flag = N_VBufPack(N_Vector x, void *buf);`

Description This routine fills the exchange buffer `buf` with the vector data in `x`.

Arguments `x` (`N_Vector`) a NVECTOR object
`buf` (`sunindextype*`) the exchange buffer to pack

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VBufPack`

`N_VBufUnpack`

Call `flag = N_VBufUnpack(N_Vector x, void *buf);`

Description This routine unpacks the data in the exchange buffer `buf` into the vector `x`.

Arguments `x` (`N_Vector`) a NVECTOR object
`buf` (`sunindextype*`) the exchange buffer to unpack

Return value Returns an `int` with value `0` for success and a non-zero value otherwise.

F2003 Name `FN_VBufUnpack`

7.1.6 NVECTOR utility functions

To aid in the creation of custom NVECTOR modules the generic NVECTOR module provides three utility functions `N_VNewEmpty`, `N_VCopyOps` and `N_VFreeEmpty`. When used in custom NVECTOR constructors and clone routines these functions will ease the introduction of any new optional vector operations to the NVECTOR API by ensuring only required operations need to be set and all operations are copied when cloning a vector.

To aid the use of arrays of NVECTOR objects, the generic NVECTOR module also provides the utility functions `N_VCloneVectorArray`, `N_VCloneVectorArrayEmpty`, and `N_VDestroyVectorArray`.

`N_VNewEmpty`

Call `v = N_VNewEmpty();`

Description The function `N_VNewEmpty` allocates a new generic NVECTOR object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

Arguments None

Return value This function returns an `N_Vector` object. If an error occurs when allocating the object, then this routine will return `NULL`.

F2003 Name `FN_VNewEmpty`

`N_VCopyOps`

Call `retval = N_VCopyOps(w, v);`

Description The function `N_VCopyOps` copies the function pointers in the `ops` structure of `w` into the `ops` structure of `v`.

Arguments `w` (`N_Vector`) the vector to copy operations from
`v` (`N_Vector`) the vector to copy operations to

Return value This returns `0` if successful and a non-zero value if either of the inputs are `NULL` or the `ops` structure of either input is `NULL`.

F2003 Name `FN_VCopyOps`

`N_VFreeEmpty`

Call `N_VFreeEmpty(v);`

Description This routine frees the generic `N_Vector` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `v` (`N_Vector`)

Return value None

F2003 Name `FN_VFreeEmpty`

`N_VCloneEmptyVectorArray`

Call `vecarray = N_VCloneEmptyVectorArray(count, w);`

Description Creates an array of `count` variables of type `N_Vector`, each of the same type as the existing `N_Vector` w. It achieves this by calling the implementation-specific `N_VCloneEmpty` operation.

Arguments `count` (`int`) the size of the vector array

`w` (`N_Vector`) the vector to clone

Return value Returns an array of `count` `N_Vector` objects if successful, or `NULL` if an error occurred while cloning.

`N_VCloneVectorArray`

Call `vecarray = N_VCloneVectorArray(count, w);`

Description Creates an array of `count` variables of type `N_Vector`, each of the same type as the existing `N_Vector` w. It achieves this by calling the implementation-specific `N_VClone` operation.

Arguments `count` (`int`) the size of the vector array

`w` (`N_Vector`) the vector to clone

Return value Returns an array of `count` `N_Vector` objects if successful, or `NULL` if an error occurred while cloning.

`N_VDestroyVectorArray`

Call `N_VDestroyVectorArray(count, w);`

Description Destroys (frees) an array of variables of type `N_Vector`. It depends on the implementation-specific `N_VDestroy` operation.

Arguments `vs` (`N_Vector*`) the array of vectors to destroy

`count` (`int`) the size of the vector array

Return value None

`N_VNewVectorArray`

Call `vecarray = N_VNewVectorArray(count);`

Description Returns an empty `N_Vector` array large enough to hold `count` `N_Vector` objects. This function is primarily meant for users of the Fortran 2003 interface.

Arguments `count` (`int`) the size of the vector array

Return value Returns a `N_Vector*` if successful, Returns `NULL` if an error occurred.

Notes Users of the Fortran 2003 interface to the `N_VManyVector` or `N_VMPIManyVector` will need this to create an array to hold the subvectors. Note that this function does restrict the the max number of subvectors usable with the `N_VManyVector` and `N_VMPIManyVector` to the max size of an `int` despite the ManyVector implementations accepting a subvector count larger than this value.

F2003 Name `FN_VNewVectorArray`

Table 7.1: Vector Identifications associated with vector kernels supplied with SUNDIALS.

Vector ID	Vector type	ID Value
SUNDIALS_NVEC_SERIAL	Serial	0
SUNDIALS_NVEC_PARALLEL	Distributed memory parallel (MPI)	1
SUNDIALS_NVEC_OPENMP	OpenMP shared memory parallel	2
SUNDIALS_NVEC_PTHREADS	PThreads shared memory parallel	3
SUNDIALS_NVEC_PARHYP	*hypre* ParHyp parallel vector	4
SUNDIALS_NVEC_PETSC	PETSc parallel vector	5
SUNDIALS_NVEC_CUDA	CUDA vector	6
SUNDIALS_NVEC_HIP	HIP vector	7
SUNDIALS_NVEC_SYCL	SYCL vector	8
SUNDIALS_NVEC_RAJA	RAJA vector	9
SUNDIALS_NVEC_OPENMPDEV	OpenMP vector with device offloading	10
SUNDIALS_NVEC_TRILINOS	Trilinos Tpetra vector	11
SUNDIALS_NVEC_MANYVECTOR	"ManyVector" vector	12
SUNDIALS_NVEC_MPIMANYVECTOR	MPI-enabled "ManyVector" vector	13
SUNDIALS_NVEC_MPIPLUSX	MPI+X vector	14
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	15

`N_VGetVecAtIndexVectorArray`

Call `v = N_VGetVecAtIndexVectorArray(vecs, index);`

Description Returns the `N_Vector` object stored in the vector array at the provided index. This function is primarily meant for users of the Fortran 2003 interface.

Arguments `vecs` (`N_Vector*`) the array of vectors to index
`index` (`int`) the index of the vector to return

Return value Returns the `N_Vector` object stored in the vector array at the provided index. Returns `NULL` if an error occurred.

F2003 Name `FN_VGetVecAtIndexVectorArray`

`N_VSetVecAtIndexVectorArray`

Call `N_VSetVecAtIndexVectorArray(vecs, index, v);`

Description Sets the `N_Vector` object stored in the vector array at the provided index. This function is primarily meant for users of the Fortran 2003 interface.

Arguments `vecs` (`N_Vector*`) the array of vectors to index
`index` (`int`) the index of the vector to return
`v` (`N_Vector`) the vector to store at the index

Return value None

F2003 Name `FN_VSetVecAtIndexVectorArray`

7.1.7 NVECTOR identifiers

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 7.1.

7.1.8 The generic NVECTOR module implementation

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);
  realtype*    (*nvgetdevicearraypointer)(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);
  int          (*nvbufsize)(N_Vector, sunindextype *);
  int          (*nvbufpack)(N_Vector, void*);
  int          (*nvbufunpack)(N_Vector, void*);
};
```

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);
}
```

Section 7.1.1 defines a complete list of all standard vector operations defined by the generic NVECTOR module. Sections 7.1.2, 7.1.3 and 7.1.4 list *optional* fused, vector array and local reduction operations, respectively.

The Fortran 2003 interface provides a `bind(C)` derived-type for the `_generic_N_Vector` and the `_generic_N_Vector_Ops` structures. Their definition is given below.

```
 type, bind(C), public :: N_Vector
  type(C_PTR), public :: content
  type(C_PTR), public :: ops
 end type N_Vector

 type, bind(C), public :: N_Vector_Ops
  type(C_FUNPTR), public :: nvgetvectorid
  type(C_FUNPTR), public :: nvclone
  type(C_FUNPTR), public :: nvcloneempty
  type(C_FUNPTR), public :: nvdestroy
  type(C_FUNPTR), public :: nvspace
  type(C_FUNPTR), public :: nvgetarraypointer
  type(C_FUNPTR), public :: nvsetarraypointer
  type(C_FUNPTR), public :: nvgetcommunicator
  type(C_FUNPTR), public :: nvgetlength
  type(C_FUNPTR), public :: nvlinearsum
  type(C_FUNPTR), public :: nvconst
  type(C_FUNPTR), public :: nvprod
  type(C_FUNPTR), public :: nvdiv
  type(C_FUNPTR), public :: nvscale
  type(C_FUNPTR), public :: nvabs
  type(C_FUNPTR), public :: nvinv
  type(C_FUNPTR), public :: nvaddconst
  type(C_FUNPTR), public :: nvdotprod
  type(C_FUNPTR), public :: nvmaxnorm
  type(C_FUNPTR), public :: nvwrmsnorm
```

```
  type(C_FUNPTR), public :: nvwrmsnormmask
  type(C_FUNPTR), public :: nvmin
  type(C_FUNPTR), public :: nvwl2norm
  type(C_FUNPTR), public :: nvl1norm
  type(C_FUNPTR), public :: nvcompare
  type(C_FUNPTR), public :: nvinvtest
  type(C_FUNPTR), public :: nvconstrmask
  type(C_FUNPTR), public :: nvminquotient
  type(C_FUNPTR), public :: nvlinearcombination
  type(C_FUNPTR), public :: nvscaleaddmulti
  type(C_FUNPTR), public :: nvdotprodmulti
  type(C_FUNPTR), public :: nvlinearsumvectorarray
  type(C_FUNPTR), public :: nvscalevectorarray
  type(C_FUNPTR), public :: nvconstvectorarray
  type(C_FUNPTR), public :: nvwrmsnormvectorarray
  type(C_FUNPTR), public :: nvwrmsnormmaskvectorarray
  type(C_FUNPTR), public :: nvscaleaddmultivectorarray
  type(C_FUNPTR), public :: nvlinearcombinationvectorarray
  type(C_FUNPTR), public :: nvdotprodlocal
  type(C_FUNPTR), public :: nvmaxnormlocal
  type(C_FUNPTR), public :: nvminlocal
  type(C_FUNPTR), public :: nvl1normlocal
  type(C_FUNPTR), public :: nvinvtestlocal
  type(C_FUNPTR), public :: nvconstrmasklocal
  type(C_FUNPTR), public :: nvminquotientlocal
  type(C_FUNPTR), public :: nvwsqrsumlocal
  type(C_FUNPTR), public :: nvwsqrsummasklocal
  type(C_FUNPTR), public :: nvbufsize
  type(C_FUNPTR), public :: nvbufpack
  type(C_FUNPTR), public :: nvbufunpack
 end type N_Vector_Ops
```

7.1.9 Implementing a custom NVECTOR

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`.

It is recommended that a user-supplied NVECTOR implementation returns the `SUNDIALS_NVEC_CUSTOM` identifier from the `N_VGetVectorID` function.

To aid in the creation of custom NVECTOR modules the generic NVECTOR module provides two utility functions `N_VNewEmpty` and `N_VCopyOps`. When used in custom NVECTOR constructors and clone routines these functions will ease the introduction of any new optional vector operations to the

NVECTOR API by ensuring only required operations need to be set and all operations are copied when cloning a vector.

7.1.9.1 Support for complex-valued vectors

While SUNDIALS itself is written under an assumption of real-valued data, it does provide limited support for complex-valued problems. However, since none of the built-in NVECTOR modules supports complex-valued data, users must provide a custom NVECTOR implementation for this task. Many of the NVECTOR routines described in Sections 7.1.1-7.1.4 above naturally extend to complex-valued vectors; however, some do not. To this end, we provide the following guidance:

- `N_VMin` and `N_VMinLocal` should return the minimum of all *real* components of the vector, i.e., $m = \min_i \text{real}(x_i)$.
- `N_VConst` (and similarly `N_VConstVectorArray`) should set the real components of the vector to the input constant, and set all imaginary components to zero, i.e., $z_i = c + 0j$, $i = 0, \ldots, n-1$.
- `N_VAddConst` should only update the real components of the vector with the input constant, leaving all imaginary components unchanged.
- `N_VWrmsNorm`, `N_VWrmsNormMask`, `N_VWSqrSumLocal` and `N_VWSqrSumMaskLocal` should assume that all entries of the weight vector `w` and the mask vector `id` are real-valued.
- `N_VDotProd` should mathematically return a complex number for complex-valued vectors; as this is not possible with SUNDIALS' current `realtype`, this routine should be set to `NULL` in the custom NVECTOR implementation.
- `N_VCompare`, `N_VConstrMask`, `N_VMinQuotient`, `N_VConstrMaskLocal` and `N_VMinQuotientLocal` are ill-defined due to the lack of a clear ordering in the complex plane. These routines should be set to `NULL` in the custom NVECTOR implementation.

While many SUNDIALS solver modules may be utilized on complex-valued data, others cannot. Specifically, although both SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT may be used with any of the IVP solvers (CVODE, CVODES, IDA, IDAS and ARKODE) for complex-valued problems, the Anderson-acceleration feature SUNNONLINSOL_FIXEDPOINT cannot be used due to its reliance on `N_VDotProd`. By this same logic, the Anderson acceleration feature within KINSOL also will not work with complex-valued vectors.

Similarly, although each package's linear solver interface (e.g., CVLS) may be used on complex-valued problems, none of the built-in SUNMATRIX or SUNLINSOL modules work. Hence a complex-valued user should provide a custom SUNLINSOL (and optionally a custom SUNMATRIX) implementation for solving linear systems, and then attach this module as normal to the package's linear solver interface.

Finally, constraint-handling features of each package cannot be used for complex-valued data, due to the issue of ordering in the complex plane discussed above with `N_VCompare`, `N_VConstrMask`, `N_VMinQuotient`, `N_VConstrMaskLocal` and `N_VMinQuotientLocal`.

We provide a simple example of a complex-valued example problem, including a custom complex-valued Fortran 2003 NVECTOR module, in the files
`examples/arkode/F2003_custom/ark_analytic_complex_f2003.f90`,
`examples/arkode/F2003_custom/fnvector_complex_mod.f90`, and
`examples/arkode/F2003_custom/test_fnvector_complex_mod.f90`.

7.2 NVECTOR functions used by IDA

In Table 7.2 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.

Table 7.2: List of vector functions usage by IDA code modules

	IDA	IDALS	IDABBDPRE	FIDA
N_VGetVectorID				
N_VGetLength		4		
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_VMaxNorm	✓			
N_VWrmsNorm	✓			
N_VMin	✓			
N_VMinQuotient	✓			
N_VConstrMask	✓			
N_VWrmsNormMask	✓			
N_VCompare	✓			
N_VLinearCombination	✓			
N_VScaleAddMulti	✓			
N_VDotProdMulti		3		
N_VLinearSumVectorArray	✓			
N_VScaleVectorArray	✓			

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.

3. The optional function N_VDotProdMulti is only used when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR. The remaining operations from Tables 7.1.2 and 7.1.3 not listed above are unused and a user-supplied NVECTOR module for IDA could omit these operations.

4. This routine is only used when an iterative or matrix iterative SUNLINSOL module is supplied to IDA.

Of the functions listed in Table 7.1.1, N_VWL2Norm, N_VL1Norm, N_VInvTest, and N_VGetCommunicator are *not* used by IDA. Therefore a user-supplied NVECTOR module for IDA could omit these functions (although some may be needed by SUNNONLINSOL or SUNLINSOL modules).

7.3 The NVECTOR_SERIAL implementation

The serial implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_SERIAL, defines the *content* field of N_Vector to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, and a boolean flag *own_data* which specifies the ownership of *data*.

```
struct _N_VectorContent_Serial {
  sunindextype length;
  booleantype own_data;
  realtype *data;
};
```

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

7.3.1 NVECTOR_SERIAL accessor macros

The following macros are provided to access the content of an NVECTOR_SERIAL vector. The suffix _S in the names denotes the serial version.

- NV_CONTENT_S

  This routine gives access to the contents of the serial vector N_Vector.

  The assignment v_cont = NV_CONTENT_S(v) sets v_cont to be a pointer to the serial N_Vector content structure.

  Implementation:

  ```
  #define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
  ```

- NV_OWN_DATA_S, NV_DATA_S, NV_LENGTH_S

  These macros give individual access to the parts of the content of a serial N_Vector.

  The assignment v_data = NV_DATA_S(v) sets v_data to be a pointer to the first component of the data for the N_Vector v. The assignment NV_DATA_S(v) = v_data sets the component array of v to be v_data by storing the pointer v_data.

  The assignment v_len = NV_LENGTH_S(v) sets v_len to be the length of v. On the other hand, the call NV_LENGTH_S(v) = len_v sets the length of v to be len_v.

  Implementation:

  ```
  #define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )
  #define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )
  #define NV_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
  ```

- NV_Ith_S

  This macro gives access to the individual components of the data array of an N_Vector.

  The assignment r = NV_Ith_S(v,i) sets r to be the value of the i-th component of v. The assignment NV_Ith_S(v,i) = r sets the value of the i-th component of v to be r.

Here i ranges from 0 to $n-1$ for a vector of length n.

Implementation:

```
#define NV_Ith_S(v,i) ( NV_DATA_S(v)[i] )
```

7.3.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3 and 7.1.4. 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 7.1.1 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.

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

`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.

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

`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`.

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

`N_VPrint_Serial`

Prototype `void N_VPrint_Serial(N_Vector v);`

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

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

`N_VPrintFile_Serial`

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

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

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

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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`N_VEnableWrmsNormMaskVectorArray_Serial`

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

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

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

`N_VEnableScaleAddMultiVectorArray_Serial`

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

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

`N_VEnableLinearCombinationVectorArray_Serial`

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

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

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_S(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_S(v,i)` within the loop.

- `N_VNewEmpty_Serial`, `N_VMake_Serial`, and `N_VCloneVectorArrayEmpty_Serial` set the field *own_data* = `SUNFALSE`. `N_VDestroy_Serial` and `N_VDestroyVectorArray_Serial` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_SERIAL implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.3.3 NVECTOR_SERIAL Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the NVECTOR_SERIAL module also includes a FORTRAN-callable function `FNVINITS(code, NEQ, IER)`, to initialize this NVECTOR_SERIAL module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type `long int`); and IER is an error return flag equal 0 for success and -1 for failure.

7.4 The NVECTOR_PARALLEL implementation

The NVECTOR_PARALLEL implementation of the NVECTOR module provided with SUNDIALS is based on MPI. It defines the *content* field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the beginning of a contiguous local data array, an MPI communicator, and a boolean flag *own_data* indicating ownership of the data array *data*.

```
struct _N_VectorContent_Parallel {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_data;
  realtype *data;
  MPI_Comm comm;
};
```

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

7.4.1 NVECTOR_PARALLEL accessor macros

The following macros are provided to access the content of a NVECTOR_PARALLEL vector. The suffix `_P` in the names denotes the distributed memory parallel version.

- `NV_CONTENT_P`

  This macro gives access to the contents of the parallel vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_P(v)` sets `v_cont` to be a pointer to the `N_Vector` content structure of type `struct _N_VectorContent_Parallel`.

  Implementation:

  ```
  #define NV_CONTENT_P(v) ( (N_VectorContent_Parallel)(v->content) )
  ```

- `NV_OWN_DATA_P`, `NV_DATA_P`, `NV_LOCLENGTH_P`, `NV_GLOBLENGTH_P`

  These macros give individual access to the parts of the content of a parallel `N_Vector`.

The assignment `v_data = NV_DATA_P(v)` sets `v_data` to be a pointer to the first component of the local data for the `N_Vector` `v`. The assignment `NV_DATA_P(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

The assignment `v_llen = NV_LOCLENGTH_P(v)` sets `v_llen` to be the length of the local part of `v`. The call `NV_LENGTH_P(v) = llen_v` sets the local length of `v` to be `llen_v`.

The assignment `v_glen = NV_GLOBLENGTH_P(v)` sets `v_glen` to be the global length of the vector `v`. The call `NV_GLOBLENGTH_P(v) = glen_v` sets the global length of `v` to be `glen_v`.

Implementation:

```
#define NV_OWN_DATA_P(v)    ( NV_CONTENT_P(v)->own_data )
#define NV_DATA_P(v)        ( NV_CONTENT_P(v)->data )
#define NV_LOCLENGTH_P(v)   ( NV_CONTENT_P(v)->local_length )
#define NV_GLOBLENGTH_P(v)  ( NV_CONTENT_P(v)->global_length )
```

- `NV_COMM_P`

  This macro provides access to the MPI communicator used by the NVECTOR_PARALLEL vectors.

  Implementation:

  ```
  #define NV_COMM_P(v) ( NV_CONTENT_P(v)->comm )
  ```

- `NV_Ith_P`

  This macro gives access to the individual components of the local data array of an `N_Vector`.

  The assignment `r = NV_Ith_P(v,i)` sets `r` to be the value of the `i`-th component of the local part of `v`. The assignment `NV_Ith_P(v,i) = r` sets the value of the `i`-th component of the local part of `v` to be `r`.

  Here i ranges from 0 to $n-1$, where n is the local length.

  Implementation:

  ```
  #define NV_Ith_P(v,i) ( NV_DATA_P(v)[i] )
  ```

7.4.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4. 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.

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

`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.

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

`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.

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

`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.

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

`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.

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

`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`.

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

`N_VGetLocalLength_Parallel`

Prototype `sunindextype N_VGetLocalLength_Parallel(N_Vector v);`

Description This function returns the local vector length.

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

`N_VPrint_Parallel`

Prototype `void N_VPrint_Parallel(N_Vector v);`

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

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

`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`.

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

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

`N_VEnableFusedOps_Parallel`

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

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

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`N_VEnableScaleAddMultiVectorArray_Parallel`

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

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

`N_VEnableLinearCombinationVectorArray_Parallel`

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

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

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the local component array via `v_data = NV_DATA_P(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_P(v,i)` within the loop.

- `N_VNewEmpty_Parallel`, `N_VMake_Parallel`, and `N_VCloneVectorArrayEmpty_Parallel` set the field *own_data* = `SUNFALSE`. `N_VDestroy_Parallel` and `N_VDestroyVectorArray_Parallel` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PARALLEL implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.4.3 NVECTOR_PARALLEL Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the NVECTOR_PARALLEL module also includes a FORTRAN-callable function `FNVINITP(COMM, code, NLOCAL, NGLOBAL, IER)`, to initialize this NVECTOR_PARALLEL module. Here `COMM` is the MPI communicator, `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `NLOCAL` and `NGLOBAL` are the local and global vector sizes, respectively (declared so as to match C type `long int`); and IER is an error return flag equal 0 for success and -1 for failure. NOTE: If the header file `sundials_config.h` defines `SUNDIALS_MPI_COMM_F2C` to be 1 (meaning the MPI implementation used to build SUNDIALS includes the `MPI_Comm_f2c` function), then `COMM` can be any valid MPI communicator. Otherwise, `MPI_COMM_WORLD` will be used, so just pass an integer value as a placeholder.

7.5 The NVECTOR_OPENMP implementation

In situations where a user has a multi-core processing unit capable of running multiple parallel threads with shared memory, SUNDIALS provides an implementation of NVECTOR using OpenMP, called NVECTOR_OPENMP, and an implementation using Pthreads, called NVECTOR_PTHREADS. Testing has shown that vectors should be of length at least $100,000$ before the overhead associated with creating and using the threads is made up by the parallelism in the vector calculations.

The OpenMP NVECTOR implementation provided with SUNDIALS, NVECTOR_OPENMP, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, a boolean flag *own_data* which specifies the ownership of *data*, and the number of threads. Operations on the vector are threaded using OpenMP.

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

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

7.5.1 NVECTOR_OPENMP accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMP vector. The suffix `_OMP` in the names denotes the OpenMP version.

- `NV_CONTENT_OMP`

  This routine gives access to the contents of the OpenMP vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_OMP(v)` sets `v_cont` to be a pointer to the OpenMP `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_OMP(v) ( (N_VectorContent_OpenMP)(v->content) )
  ```

- `NV_OWN_DATA_OMP`, `NV_DATA_OMP`, `NV_LENGTH_OMP`, `NV_NUM_THREADS_OMP`

  These macros give individual access to the parts of the content of a OpenMP `N_Vector`.

  The assignment `v_data = NV_DATA_OMP(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_OMP(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_len = NV_LENGTH_OMP(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_OMP(v) = len_v` sets the length of `v` to be `len_v`.

  The assignment `v_num_threads = NV_NUM_THREADS_OMP(v)` sets `v_num_threads` to be the number of threads from `v`. On the other hand, the call `NV_NUM_THREADS_OMP(v) = num_threads_v` sets the number of threads for `v` to be `num_threads_v`.

  Implementation:

  ```
  #define NV_OWN_DATA_OMP(v) ( NV_CONTENT_OMP(v)->own_data )
  #define NV_DATA_OMP(v) ( NV_CONTENT_OMP(v)->data )
  #define NV_LENGTH_OMP(v) ( NV_CONTENT_OMP(v)->length )
  #define NV_NUM_THREADS_OMP(v) ( NV_CONTENT_OMP(v)->num_threads )
  ```

- `NV_Ith_OMP`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_OMP(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_OMP(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_OMP(v,i) ( NV_DATA_OMP(v)[i] )
  ```

7.5.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4. 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 7.1.1 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.

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

`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.

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

`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`.

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

`N_VPrint_OpenMP`

Prototype `void N_VPrint_OpenMP(N_Vector v)`

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

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

`N_VPrintFile_OpenMP`

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

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

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

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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`N_VEnableScaleAddMultiVectorArray_OpenMP`

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

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

`N_VEnableLinearCombinationVectorArray_OpenMP`

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

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

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_OMP(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_OMP(v,i)` within the loop.

- `N_VNewEmpty_OpenMP`, `N_VMake_OpenMP`, and `N_VCloneVectorArrayEmpty_OpenMP` set the field *own_data* = `SUNFALSE`. `N_VDestroy_OpenMP` and `N_VDestroyVectorArray_OpenMP` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_OPENMP implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.5.3 NVECTOR_OPENMP Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the NVECTOR_OPENMP module also includes a FORTRAN-callable function `FNVINITOMP(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type `long int`); NUMTHREADS is the number of threads; and IER is an error return flag equal 0 for success and -1 for failure.

7.6 The NVECTOR_PTHREADS implementation

In situations where a user has a multi-core processing unit capable of running multiple parallel threads with shared memory, SUNDIALS provides an implementation of NVECTOR using OpenMP, called NVECTOR_OPENMP, and an implementation using Pthreads, called NVECTOR_PTHREADS. Testing has shown that vectors should be of length at least $100,000$ before the overhead associated with creating and using the threads is made up by the parallelism in the vector calculations.

The Pthreads NVECTOR implementation provided with SUNDIALS, denoted NVECTOR_PTHREADS, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, a boolean flag *own_data* which specifies the ownership of *data*, and the number of threads. Operations on the vector are threaded using POSIX threads (Pthreads).

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

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

7.6.1 NVECTOR_PTHREADS accessor macros

The following macros are provided to access the content of an NVECTOR_PTHREADS vector. The suffix `_PT` in the names denotes the Pthreads version.

- `NV_CONTENT_PT`

  This routine gives access to the contents of the Pthreads vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_PT(v)` sets `v_cont` to be a pointer to the Pthreads `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_PT(v) ( (N_VectorContent_Pthreads)(v->content) )
  ```

- `NV_OWN_DATA_PT`, `NV_DATA_PT`, `NV_LENGTH_PT`, `NV_NUM_THREADS_PT`

  These macros give individual access to the parts of the content of a Pthreads `N_Vector`.

  The assignment `v_data = NV_DATA_PT(v)` sets `v_data` to be a pointer to the first component of the data for the `N_Vector v`. The assignment `NV_DATA_PT(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_len = NV_LENGTH_PT(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_PT(v) = len_v` sets the length of `v` to be `len_v`.

  The assignment `v_num_threads = NV_NUM_THREADS_PT(v)` sets `v_num_threads` to be the number of threads from `v`. On the other hand, the call `NV_NUM_THREADS_PT(v) = num_threads_v` sets the number of threads for `v` to be `num_threads_v`.

Implementation:

```
#define NV_OWN_DATA_PT(v) ( NV_CONTENT_PT(v)->own_data )

#define NV_DATA_PT(v) ( NV_CONTENT_PT(v)->data )

#define NV_LENGTH_PT(v) ( NV_CONTENT_PT(v)->length )

#define NV_NUM_THREADS_PT(v) ( NV_CONTENT_PT(v)->num_threads )
```

- `NV_Ith_PT`

  This macro gives access to the individual components of the data array of an `N_Vector`.

  The assignment `r = NV_Ith_PT(v,i)` sets `r` to be the value of the `i`-th component of `v`. The assignment `NV_Ith_PT(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

  Here i ranges from 0 to $n-1$ for a vector of length n.

  Implementation:

  ```
  #define NV_Ith_PT(v,i) ( NV_DATA_PT(v)[i] )
  ```

7.6.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4. 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 7.1.1 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.

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

`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.

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

`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`.

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

`N_VPrint_Pthreads`

Prototype `void N_VPrint_Pthreads(N_Vector v)`

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

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

`N_VPrintFile_Pthreads`

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

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

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

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

`N_VEnableFusedOps_Pthreads`

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

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

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`N_VEnableScaleAddMultiVectorArray_Pthreads`

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

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

`N_VEnableLinearCombinationVectorArray_Pthreads`

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

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

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = NV_DATA_PT(v)` and then access `v_data[i]` within the loop than it is to use `NV_Ith_PT(v,i)` within the loop.

- `N_VNewEmpty_Pthreads`, `N_VMake_Pthreads`, and `N_VCloneVectorArrayEmpty_Pthreads` set the field *own_data* = `SUNFALSE`. `N_VDestroy_Pthreads` and `N_VDestroyVectorArray_Pthreads` will not attempt to free the pointer *data* for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PTHREADS implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.6.3 NVECTOR_PTHREADS Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the NVECTOR_PTHREADS module also includes a FORTRAN-callable function `FNVINITPTS(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NEQ is the problem size (declared so as to match C type `long int`); NUMTHREADS is the number of threads; and IER is an error return flag equal 0 for success and -1 for failure.

7.7 The NVECTOR_PARHYP implementation

The NVECTOR_PARHYP implementation of the NVECTOR module provided with SUNDIALS is a wrapper around *hypre*'s ParVector class. Most of the vector kernels simply call *hypre* vector operations. The implementation defines the *content* field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to an object of type `HYPRE_ParVector`, an MPI communicator, and a boolean flag *own_parvector* indicating ownership of the *hypre* parallel vector object x.

```
struct _N_VectorContent_ParHyp {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_parvector;
  MPI_Comm comm;
  HYPRE_ParVector x;
};
```

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

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

7.7.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VSetArrayPointer` and `N_VGetArrayPointer`, because accessing raw vector data is handled by low-level *hypre* functions. As such, this vector is not available for use with SUNDIALS Fortran interfaces. When access to raw vector data is needed, one should extract the *hypre* vector first, and then use *hypre* methods to access the data. Usage examples of NVECTOR_PARHYP are provided in the `cvAdvDiff_non_ph.c` example program for CVODE [35] and the `ark_diurnal_kry_ph.c` example program for ARKODE [42].

The names of parhyp methods are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR_PARHYP provides the following additional user-callable routines:

`N_VNewEmpty_ParHyp`

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

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

`N_VMake_ParHyp`

Prototype `N_Vector N_VMake_ParHyp(HYPRE_ParVector x)`

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

`N_VGetVector_ParHyp`

Prototype `HYPRE_ParVector N_VGetVector_ParHyp(N_Vector v)`

Description This function returns the underlying *hypre* vector.

`N_VCloneVectorArray_ParHyp`

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

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

`N_VCloneVectorArrayEmpty_ParHyp`

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

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

`N_VDestroyVectorArray_ParHyp`

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

Description This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_ParHyp` or with `N_VCloneVectorArrayEmpty_ParHyp`.

`N_VPrint_ParHyp`

Prototype `void N_VPrint_ParHyp(N_Vector v)`

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

`N_VPrintFile_ParHyp`

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

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

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

`N_VEnableFusedOps_ParHyp`

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

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

`N_VEnableLinearCombination_ParHyp`

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

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

`N_VEnableScaleAddMulti_ParHyp`

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

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

`N_VEnableDotProdMulti_ParHyp`

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

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

`N_VEnableLinearSumVectorArray_ParHyp`

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

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

`N_VEnableScaleVectorArray_ParHyp`

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

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

N_VEnableConstVectorArray_ParHyp

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

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

N_VEnableWrmsNormVectorArray_ParHyp

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

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

N_VEnableWrmsNormMaskVectorArray_ParHyp

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

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

N_VEnableScaleAddMultiVectorArray_ParHyp

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

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

N_VEnableLinearCombinationVectorArray_ParHyp

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

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

Notes

- When there is a need to access components of an N_Vector_ParHyp, v, it is recommended to extract the *hypre* vector via `x_vec = N_VGetVector_ParHyp(v)` and then access components using appropriate *hypre* functions.

- N_VNewEmpty_ParHyp, N_VMake_ParHyp, and N_VCloneVectorArrayEmpty_ParHyp set the field *own_parvector* to SUNFALSE. N_VDestroy_ParHyp and N_VDestroyVectorArray_ParHyp will not attempt to delete an underlying *hypre* vector for any N_Vector with *own_parvector* set to SUNFALSE. In such a case, it is the user's responsibility to delete the underlying vector.

- To maximize efficiency, vector operations in the NVECTOR_PARHYP implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.8 The NVECTOR_PETSC implementation

The NVECTOR_PETSC module is an NVECTOR wrapper around the PETSc vector. It defines the *content* field of a `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the PETSc vector, an MPI communicator, and a boolean flag *own_data* indicating ownership of the wrapped PETSc vector.

```
struct _N_VectorContent_Petsc {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_data;
  Vec *pvec;
  MPI_Comm comm;
};
```

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

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

7.8.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with SUNDIALS Fortran interfaces. When access to raw vector data is needed, it is recommended to extract the PETSc vector first, and then use PETSc methods to access the data. Usage examples of NVECTOR_PETSC are provided in example programs for IDA [34].

The names of vector operations are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix `_Petsc` (e.g. `N_VDestroy_Petsc`). The module NVECTOR_PETSC provides the following additional user-callable routines:

`N_VNewEmpty_Petsc`

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

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped PETSc vector set to (`NULL`). It is used by the `N_VMake_Petsc` and `N_VClone_Petsc` implementations.

`N_VMake_Petsc`

Prototype `N_Vector N_VMake_Petsc(Vec *pvec)`

Description This function creates and allocates memory for an NVECTOR_PETSC wrapper around a user-provided PETSc vector. It does *not* allocate memory for the vector `pvec` itself.

`N_VGetVector_Petsc`

Prototype `Vec *N_VGetVector_Petsc(N_Vector v)`

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

`N_VCloneVectorArray_Petsc`

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

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

`N_VCloneVectorArrayEmpty_Petsc`

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

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

`N_VDestroyVectorArray_Petsc`

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

Description This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Petsc` or with `N_VCloneVectorArrayEmpty_Petsc`.

`N_VPrint_Petsc`

Prototype `void N_VPrint_Petsc(N_Vector v)`

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

`N_VPrintFile_Petsc`

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

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

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

`N_VEnableFusedOps_Petsc`

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

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

`N_VEnableLinearCombination_Petsc`

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

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

`N_VEnableScaleAddMulti_Petsc`

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

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

`N_VEnableDotProdMulti_Petsc`

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

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

`N_VEnableLinearSumVectorArray_Petsc`

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

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

`N_VEnableScaleVectorArray_Petsc`

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

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

`N_VEnableConstVectorArray_Petsc`

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

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

`N_VEnableWrmsNormVectorArray_Petsc`

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

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

`N_VEnableWrmsNormMaskVectorArray_Petsc`

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

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

`N_VEnableScaleAddMultiVectorArray_Petsc`

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

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

`N_VEnableLinearCombinationVectorArray_Petsc`

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

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

Notes

- When there is a need to access components of an `N_Vector_Petsc`, `v`, it is recommeded to extract the PETSc vector via `x_vec = N_VGetVector_Petsc(v)` and then access components using appropriate PETSc functions.

- The functions `N_VNewEmpty_Petsc`, `N_VMake_Petsc`, and `N_VCloneVectorArrayEmpty_Petsc` set the field *own_data* to `SUNFALSE`. `N_VDestroy_Petsc` and `N_VDestroyVectorArray_Petsc` will not attempt to free the pointer *pvec* for any `N_Vector` with *own_data* set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *pvec* pointer.

- To maximize efficiency, vector operations in the NVECTOR_PETSC implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.9 The NVECTOR_CUDA implementation

The NVECTOR_CUDA module is an NVECTOR implementation in the CUDA language. The module allows for SUNDIALS vector kernels to run on NVIDIA 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 vector content layout is as follows:

```
struct _N_VectorContent_Cuda
{
  sunindextype       length;
  booleantype        own_exec;
  booleantype        own_helper;
  SUNMemory          host_data;
  SUNMemory          device_data;
  SUNCudaExecPolicy* stream_exec_policy;
  SUNCudaExecPolicy* reduce_exec_policy;
  SUNMemoryHelper    mem_helper;
  void*              priv; /* 'private' data */
};

typedef struct _N_VectorContent_Cuda *N_VectorContent_Cuda;
```

The content members are the vector length (size), ownership flags for the `*_exec_policy` fields and the `mem_helper` field, `SUNMemory` objects for the vector data on the host and the device, pointers to

SUNCudaExecPolicy implementations that control how the CUDA kernels are launched for streaming and reduction vector kernels, a SUNMemoryHelper object, and a private data structure which holds additonal members that should not be accessed directly.

When instantiated with N_VNew_Cuda, the underlying data will be allocated 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.

To use the NVECTOR_CUDA module, the header file to include is nvector_cuda.h, and the library to link to is libsundials_nveccuda.*lib*. The extension *.lib* is typically .so for shared libraries and .a for static libraries.

7.9.1 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_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_VSetHostArrayPointer_Cuda

Prototype `realtype *N_VSetHostArrayPointer_Cuda(N_Vector v)`

Description This function sets the pointer to the vector data on the host. The existing pointer *will not* be freed first.

N_VSetDeviceArrayPointer_Cuda

Prototype `realtype *N_VSetDeviceArrayPointer_Cuda(N_Vector v)`

Description This function sets pointer to the vector data on the device. The existing pointer *will not* be freed first.

N_VIsManagedMemory_Cuda

Prototype `booleantype *N_VIsManagedMemory_Cuda(N_Vector v)`

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

The NVECTOR_CUDA module defines implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3 and 7.1.4, except for N_VSetArrayPointer and N_VGetArrayPointer unless managed memory is used. As such, this vector can only be used with the SUNDIALS Fortran interfaces, and the SUNDIALS direct solvers and preconditioners when using managed memory. The NVECTOR_CUDA module provides separate functions to access data on the host and on the device for the unmanaged memory use case. 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 [35].

The names of vector operations are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix _Cuda (e.g. N_VDestroy_Cuda). The module NVECTOR_CUDA provides the following functions:

`N_VNew_Cuda`

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.

`N_VNewManaged_Cuda`

Prototype `N_Vector N_VNewManaged_Cuda(sunindextype length)`

Description This function creates and allocates memory for a CUDA `N_Vector`. The vector data array is allocated in managed memory.

`N_VNewWithMemHelp_Cuda`

Prototype `N_Vector N_VNewWithMemHelp_Cuda(sunindextype length, booleantype use_managed_mem, SUNMemoryHelper helper);`

Description This function creates an NVECTOR_CUDA which will use the `SUNMemoryHelper` object to allocate memory. If `use_managed_memory` is 0, then unmanaged memory is used, otherwise managed memory is used.

`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`

Prototype `N_Vector N_VMake_Cuda(sunindextype length, realtype *h_data, realtype *dev_data)`

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.

`N_VMakeManaged_Cuda`

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.

`N_VMakeWithManagedAllocator_Cuda`

Prototype `N_Vector N_VMakeWithManagedAllocator_Cuda(sunindextype length, void* (*allocfn)(size_t size), void (*freefn)(void* ptr));`

Description This function creates an NVECTOR_CUDA with a user-supplied memory allocator. It requires the user to provide a corresponding free function as well. The memory allocated by the allocator function must behave like CUDA managed memory.

This function is deprecated and will be removed in the next major release. Use `N_VNewWithMemHelp_Cuda` instead.

The module NVECTOR_CUDA also provides the following user-callable routines:

`N_VSetKernelExecPolicy_Cuda`

Prototype `void N_VSetKernelExecPolicy_Cuda(N_Vector v, SUNCudaExecPolicy* stream_exec_policy, SUNCudaExecPolicy* reduce_exec_policy);`

Description This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction CUDA kernels. By default the vector is setup to use the `SUNCudaThreadDirectExecPolicy` and `SUNCudaBlockReduceExecPolicy`. Any custom execution policy for reductions must ensure that the grid dimensions (number of thread blocks) is a multiple of the CUDA warp size (32). See section 7.9.2 below for more information about the `SUNCudaExecPolicy` class.

Note: All vectors used in a single instance of a SUNDIALS *solver must use the same execution policy. It is* ***strongly recommended*** *that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors.*

`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. It is* ***strongly recommended*** *that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors.*

This function will be removed in the next major release, user should utilize the `N_VSetKernelExec...icy_Cud` function instead.

`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 operations in the CUDA vector. The return value is `0` for success and `-1` if the input vector or its `ops` structure are `NULL`.

`N_VEnableLinearCombination_Cuda`

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

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

`N_VEnableScaleAddMulti_Cuda`

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

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

`N_VEnableDotProdMulti_Cuda`

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

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

`N_VEnableLinearSumVectorArray_Cuda`

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

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

`N_VEnableScaleVectorArray_Cuda`

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

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

`N_VEnableConstVectorArray_Cuda`

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

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

`N_VEnableWrmsNormVectorArray_Cuda`

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

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

`N_VEnableWrmsNormMaskVectorArray_Cuda`

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

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

`N_VEnableScaleAddMultiVectorArray_Cuda`

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

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

`N_VEnableLinearCombinationVectorArray_Cuda`

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

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

Notes

- When there is a need to access components of an `N_Vector_Cuda`, `v`, it is recommeded to use functions `N_VGetDeviceArrayPointer_Cuda` or `N_VGetHostArrayPointer_Cuda`. However, when using managed memory, the function `N_VGetArrayPointer` may also be used.
- Performance is better if the `SUNMemoryHelper` provided supports `SUNMEMTYPE_PINNED`; the default `SUNMemoryHelper` does provide this support. In the case that it does, then the buffers used for reductions will be allocated as pinned memory.
- To maximize efficiency, vector operations in the NVECTOR_CUDA implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.9.2 The SUNCudaExecPolicy Class

In order to provide maximum flexibility to users, the CUDA kernel execution parameters used by kernels within SUNDIALS are defined by objects of the `sundials::CudaExecPolicy` abstract class type (this class can be accessed in the global namespace as `SUNCudaExecPolicy`). Thus, users may provide custom execution policies that fit the needs of their problem. The `sundials::CudaExecPolicy` is defined in the header file `sundials_cuda_policies.hpp`, and is as follows:

```
class CudaExecPolicy
{
public:
```

```
  virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
  virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
  virtual cudaStream_t stream() const = 0;
  virtual CudaExecPolicy* clone() const = 0;
  virtual ~CudaExecPolicy() {}
};
```

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided `sundials::CudaThreadDirectExecPolicy` (aka in the global namespace as `SUNCudaThreadDirectExecPolicy`) class is a good example of a what a custom execution policy may look like:

```
class CudaThreadDirectExecPolicy : public CudaExecPolicy
{
public:
  CudaThreadDirectExecPolicy(const size_t blockDim, const cudaStream_t stream = 0)
    : blockDim_(blockDim), stream_(stream)
  {}

  CudaThreadDirectExecPolicy(const CudaThreadDirectExecPolicy& ex)
    : blockDim_(ex.blockDim_), stream_(ex.stream_)
  {}

  virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const
  {
    return (numWorkUnits + blockSize() - 1) / blockSize();
  }

  virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const
  {
    return blockDim_;
  }

  virtual cudaStream_t stream() const
  {
    return stream_;
  }

  virtual CudaExecPolicy* clone() const
  {
    return static_cast<CudaExecPolicy*>(new CudaThreadDirectExecPolicy(*this));
  }

private:
  const cudaStream_t stream_;
  const size_t blockDim_;
};
```

In total, SUNDIALS provides 3 execution policies:

1. `SUNCudaThreadDirectExecPolicy(const size_t blockDim, const cudaStream_t stream = 0)` maps each CUDA thread to a work unit. The number of threads per block (blockDim) can be set to anything. The grid size will be calculated so that there are enough threads for one thread per element. If a CUDA stream is provided, it will be used to execute the kernel.

2. `SUNCudaGridStrideExecPolicy(const size_t blockDim, const size_t gridDim, const cudaStream_t stream = 0)` is for kernels that use grid stride loops. The number of threads per block (blockDim) can be set to anything. The number of blocks (gridDim) can be set to anything. If a CUDA stream is provided, it will be used to execute the kernel.

3. `SUNCudaBlockReduceExecPolicy(const size_t blockDim, const size_t gridDim, const cudaStream_t stream = 0)` is for kernels performing a reduction across individual thread blocks. The number of threads per block (blockDim) can be set to any valid multiple of the CUDA warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a CUDA stream is provided, it will be used to execute the kernel.

For example, a policy that uses 128 threads per block and a user provided stream can be created like so:

```
cudaStream_t stream;
cudaStreamCreate(&stream);
SUNCudaThreadDirectExecPolicy thread_direct(128, stream);
```

These default policy objects can be reused for multiple SUNDIALS data structures since they do not hold any modifiable state information.

7.10 The NVECTOR_HIP implementation

The NVECTOR_HIP module is an NVECTOR implementation using the AMD ROCm HIP library. The module allows for SUNDIALS vector kernels to run on AMD or NVIDIA GPU devices. It is intended for users who are already familiar with HIP and GPU programming. Building this vector module requires the HIP-clang compiler. The vector content layout is as follows:

```
struct _N_VectorContent_Hip
{
  sunindextype       length;
  booleantype        own_exec;
  booleantype        own_helper;
  SUNMemory          host_data;
  SUNMemory          device_data;
  SUNHipExecPolicy*  stream_exec_policy;
  SUNHipExecPolicy*  reduce_exec_policy;
  SUNMemoryHelper    mem_helper;
  void*              priv; /* 'private' data */
};

typedef struct _N_VectorContent_Hip *N_VectorContent_Hip;
```

The content members are the vector length (size), a boolean flag that signals if the vector owns the data (i.e. it is in charge of freeing the data), pointers to vector data on the host and the device, pointers to `SUNHipExecPolicy` implementations that control how the HIP kernels are launched for streaming and reduction vector kernels, and a private data structure which holds additional members that should not be accessed directly.

When instantiated with `N_VNew_Hip`, the underlying data will be allocated memory on both the host and the device. Alternatively, a user can provide host and device data arrays by using the `N_VMake_Hip` constructor. To use HIP managed memory, the constructors `N_VNewManaged_Hip` and `N_VMakeManaged_Hip` are provided. Details on each of these constructors are provided below.

To use the NVECTOR_HIP module, the header file to include is `nvector_hip.h`, and the library to link to is `libsundials_nvechip.`*`lib`*. The extension *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

7.10.1 NVECTOR_HIP functions

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

`N_VGetHostArrayPointer_Hip`

Prototype `realtype *N_VGetHostArrayPointer_Hip(N_Vector v)`

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

`N_VGetDeviceArrayPointer_Hip`

Prototype `realtype *N_VGetDeviceArrayPointer_Hip(N_Vector v)`

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

`N_VIsManagedMemory_Hip`

Prototype `booleantype *N_VIsManagedMemory_Hip(N_Vector v)`

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

The NVECTOR_HIP module defines implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3 and 7.1.4, except for `N_VSetArrayPointer`. The names of vector operations are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix `_Hip` (e.g. `N_VDestroy_Hip`). The module NVECTOR_HIP provides the following functions:

`N_VNew_Hip`

Prototype `N_Vector N_VNew_Hip(sunindextype length)`

Description This function creates an empty HIP `N_Vector` with the data pointers set to `NULL`.

`N_VNewManaged_Hip`

Prototype `N_Vector N_VNewManaged_Hip(sunindextype length)`

Description This function creates and allocates memory for a HIP `N_Vector`. The vector data array is allocated in managed memory.

`N_VNewEmpty_Hip`

Prototype `N_Vector N_VNewEmpty_Hip()`

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped HIP vector set to `NULL`. It is used by the `N_VNew_Hip`, `N_VMake_Hip`, and `N_VClone_Hip` implementations.

`N_VMake_Hip`

Prototype `N_Vector N_VMake_Hip(sunindextype length, realtype *h_data, realtype *dev_data)`

Description This function creates an NVECTOR_HIP with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself.

`N_VMakeManaged_Hip`

Prototype `N_Vector N_VMakeManaged_Hip(sunindextype length, realtype *vdata)`

Description This function creates an NVECTOR_HIP with a user-supplied managed memory data array. This function does not allocate memory for data itself.

The module NVECTOR_HIP also provides the following user-callable routines:

`N_VSetKernelExecPolicy_Hip`

Prototype
```
void N_VSetKernelExecPolicy_Hip(N_Vector v,
                                SUNHipExecPolicy* stream_exec_policy,
                                SUNHipExecPolicy* reduce_exec_policy);
```

Description This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction HIP kernels. By default the vector is setup to use the `SUNHipThreadDirectExecPolicy` and `SUNHipBlockReduceExecPolicy`. Any custom execution policy for reductions must ensure that the grid dimensions (number of thread blocks) is a multiple of the HIP warp size (64 when targeting AMD GPUs and 32 when targing NVIDIA GPUs). See section 7.10.2 below for more information about the `SUNHipExecPolicy` class.

Note: All vectors used in a single instance of a SUNDIALS *solver must use the same execution policy. It is* ***strongly recommended*** *that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors.*

`N_VCopyToDevice_Hip`

Prototype `void N_VCopyToDevice_Hip(N_Vector v)`

Description This function copies host vector data to the device.

`N_VCopyFromDevice_Hip`

Prototype `void N_VCopyFromDevice_Hip(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VPrint_Hip`

Prototype `void N_VPrint_Hip(N_Vector v)`

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

`N_VPrintFile_Hip`

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

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

By default all fused and vector array operations are disabled in the NVECTOR_HIP 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_Hip`, 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_Hip` will have the default settings for the NVECTOR_HIP module.

`N_VEnableFusedOps_Hip`

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

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

`N_VEnableLinearCombination_Hip`

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

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

`N_VEnableScaleAddMulti_Hip`

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

`N_VEnableDotProdMulti_Hip`

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

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

`N_VEnableLinearSumVectorArray_Hip`

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

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

`N_VEnableScaleVectorArray_Hip`

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

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

`N_VEnableConstVectorArray_Hip`

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

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

`N_VEnableWrmsNormVectorArray_Hip`

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

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

`N_VEnableWrmsNormMaskVectorArray_Hip`

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

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

`N_VEnableScaleAddMultiVectorArray_Hip`

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

`N_VEnableLinearCombinationVectorArray_Hip`

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

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the HIP 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_Hip`, `v`, it is recommended to use functions `N_VGetDeviceArrayPointer_Hip` or `N_VGetHostArrayPointer_Hip`. However, when using managed memory, the function `N_VGetArrayPointer` may also be used.
- To maximize efficiency, vector operations in the NVECTOR_HIP implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.10.2 The SUNHipExecPolicy Class

In order to provide maximum flexibility to users, the HIP kernel execution parameters used by kernels within SUNDIALS are defined by objects of the `sundials::HipExecPolicy` abstract class type (this class can be accessed in the global namespace as `SUNHipExecPolicy`). Thus, users may provide custom execution policies that fit the needs of their problem. The `sundials::HipExecPolicy` is defined in the header file `sundials_hip_policies.hpp`, and is as follows:

```
class HipExecPolicy
{
public:
  virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
  virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
  virtual hipStream_t stream() const = 0;
```

```
  virtual HipExecPolicy* clone() const = 0;
  virtual ~HipExecPolicy() {}
};
```

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided `sundials::HipThreadDirectExecPolicy` (aka in the global namespace as `SUNHipThreadDirectExecPolicy`) class is a good example of a what a custom execution policy may look like:

```
class HipThreadDirectExecPolicy : public HipExecPolicy
{
public:
  HipThreadDirectExecPolicy(const size_t blockDim, const hipStream_t stream = 0)
    : blockDim_(blockDim), stream_(stream)
  {}

  HipThreadDirectExecPolicy(const HipThreadDirectExecPolicy& ex)
    : blockDim_(ex.blockDim_), stream_(ex.stream_)
  {}

  virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const
  {
    return (numWorkUnits + blockSize() - 1) / blockSize();
  }

  virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const
  {
    return blockDim_;
  }

  virtual hipStream_t stream() const
  {
    return stream_;
  }

  virtual HipExecPolicy* clone() const
  {
    return static_cast<HipExecPolicy*>(new HipThreadDirectExecPolicy(*this));
  }

private:
  const hipStream_t stream_;
  const size_t blockDim_;
};
```

In total, SUNDIALS provides 3 execution policies:

1. `SUNHipThreadDirectExecPolicy(const size_t blockDim, const hipStream_t stream = 0)` maps each HIP thread to a work unit. The number of threads per block (blockDim) can be set to anything. The grid size will be calculated so that there are enough threads for one thread per element. If a HIP stream is provided, it will be used to execute the kernel.

2. `SUNHipGridStrideExecPolicy(const size_t blockDim, const size_t gridDim, const hipStream_t stream = 0)` is for kernels that use grid stride loops. The number of threads per block (blockDim) can be set to anything. The number of blocks (gridDim) can be set to anything. If a HIP stream is provided, it will be used to execute the kernel.

3. `SUNHipBlockReduceExecPolicy(const size_t blockDim, const size_t gridDim, const hipStream_t stream = 0)` is for kernels performing a reduction across individual thread blocks. The number of threads per block (blockDim) can be set to any valid multiple of the HIP warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a HIP stream is provided, it will be used to execute the kernel.

For example, a policy that uses 128 threads per block and a user provided stream can be created like so:

```
hipStream_t stream;
hipStreamCreate(&stream);
SUNHipThreadDirectExecPolicy thread_direct(128, stream);
```

These default policy objects can be reused for multiple SUNDIALS data structures since they do not hold any modifiable state information.

7.11 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 AMD or NVIDIA 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 either the NVIDIA CUDA programming environment, or the AMD ROCm HIP programming environment. When using the AMD ROCm HIP environment, the HIP-clang compiler must be utilized. Users can select which backend (CUDA or HIP) to compile with by setting the `SUNDIALS_RAJA_BACKENDS` CMake variable to either CUDA or HIP. Besides the CUDA and HIP backends, RAJA has other backends such as serial, OpenMP, and OpenACC. These backends are not used in this SUNDIALS release.

The vector content layout is as follows:

```
struct _N_VectorContent_Raja
{
  sunindextype    length;
  booleantype     own_helper;
  SUNMemory       host_data;
  SUNMemory       device_data;
  SUNMemoryHelper mem_helper;
  void*           priv; /* 'private' data */
};
```

The content members are the vector length (size), a boolean flag that signals if the vector owns the memory helper, `SUNMemory` objects for vector data on the host and the device, a `SUNMemoryHelper` object and a private data structure which holds the memory management type, which should not be accessed directly.

When instantiated with `N_VNew_Raja`, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the `N_VMake_Raja` constructor. To use managed memory, the constructors `N_VNewManaged_Raja` and `N_VMakeManaged_Raja` are provided. Details on each of these constructors are provided below.

The header file to include when using this module is `nvector_raja.h`. The installed module library to link to are `libsundials_nveccudaraja.`*`lib`* when using the CUDA backend and `libsundials_nvechipraja.`*`lib`* when using the HIP backend. The extension *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

7.11.1 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_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_VSetHostArrayPointer_Raja`

Prototype `realtype *N_VSetHostArrayPointer_Raja(N_Vector v)`

Description This function sets the pointer to the vector data on the host. The existing pointer *will not* be freed first.

`N_VSetDeviceArrayPointer_Raja`

Prototype `realtype *N_VSetDeviceArrayPointer_Raja(N_Vector v)`

Description This function sets pointer to the vector data on the device. The existing pointer *will not* be freed first.

`N_VIsManagedMemory_Raja`

Prototype `booleantype *N_VIsManagedMemory_Raja(N_Vector v)`

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

The NVECTOR_RAJA module defines the implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VDotProdMulti`, `N_VWrmsNormVectorArray`, and `N_VWrmsNormMaskVectorArray` as support for arrays of reduction vectors is not yet supported in RAJA. These function will be added to the NVECTOR_RAJA implementation in the future. Additionally the vector operations `N_VGetArrayPointer` and `N_VSetArrayPointer` are not provided by the RAJA vector unless managed memory is used. 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 [35].

The names of vector operations are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix `_Raja` (e.g. `N_VDestroy_Raja`). The module NVECTOR_RAJA provides the following additional user-callable routines:

`N_VNew_Raja`

Prototype `N_Vector N_VNew_Raja(sunindextype length)`

Description This function creates and allocates memory for a RAJA `N_Vector`. The vector data array is allocated on both the host and device.

`N_VNewWithMemHelp_Raja`

Prototype `N_Vector N_VNewWithMemHelp_Raja(sunindextype length, booleantype use_managed_mem, SUNMemoryHelper helper);`

Description This function creates an NVECTOR_RAJA which will use the `SUNMemoryHelper` object to allocate memory. If `use_managed_memory` is 0, then unmanaged memory is used, otherwise managed memory is used.

`N_VNewManaged_Raja`

Prototype `N_Vector N_VNewManaged_Raja(sunindextype length)`

Description This function creates and allocates memory for a RAJA `N_Vector`. The vector data array is allocated in managed memory.

`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(sunindextype length, realtype *h_data, realtype *dev_data)`

Description This function creates an NVECTOR_RAJA with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself.

`N_VMakeManaged_Raja`

Prototype `N_Vector N_VMakeManaged_Raja(sunindextype length, realtype *vdata)`

Description This function creates an NVECTOR_RAJA with a user-supplied managed memory data array. This function does not allocate memory for data itself.

`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 recommended to use functions `N_VGetDeviceArrayPointer_Raja` or `N_VGetHostArrayPointer_Raja`. However, when using managed memory, the function `N_VGetArrayPointer` may also be used.
- To maximize efficiency, vector operations in the NVECTOR_RAJA implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.12 The NVECTOR_SYCL implementation

The NVECTOR_SYCL module is an experimental NVECTOR implementation using the SYCL abstraction layer. At present the only supported SYCL compiler is the DPC++ (Intel oneAPI) compiler. This module allows for SUNDIALS vector kernels to run on Intel GPU devices. The module is intended for users who are already familiar with SYCL and GPU programming.

The vector content layout is as follows:

```
struct _N_VectorContent_Sycl
{
   sunindextype       length;
   booleantype        own_exec;
   booleantype        own_helper;
   SUNMemory          host_data;
   SUNMemory          device_data;
   SUNSyclExecPolicy* stream_exec_policy;
   SUNSyclExecPolicy* reduce_exec_policy;
   SUNMemoryHelper    mem_helper;
   sycl::queue*       queue;
   void*              priv; /* 'private' data */
};

typedef struct _N_VectorContent_Sycl *N_VectorContent_Sycl;
```

The content members are the vector length (size), boolean flags that indicate if the vector owns the execution policies and memory helper objects (i.e., it is in charge of freeing the objects), `SUNMemory` objects for the vector data on the host and device, pointers to execution policies that control how streaming and reduction kernels are launched, a `SUNMemoryHelper` for performing memory operations,

the SYCL queue, and a private data structure which holds additional members that should not be accessed directly.

When instantiated with `N_VNew_Sycl()`, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the `N_VMake_Sycl()` constructor. To use managed (shared) memory, the constructors `N_VNewManaged_Sycl()` and `N_VMakeManaged_Sycl()` are provided. Additionally, a user-defined `SUNMemoryHelper` for allocating/freeing data can be provided with the constructor `N_VNewWithMemHelp_Sycl()`. Details on each of these constructors are provided below.

The header file to include when using this is `nvector_sycl.h`. The installed module library to link to is `libsundials_nvecsycl.lib`. The extension `.lib` is typically `.so` for shared libraries `.a` for static libraries.

7.12.1 NVECTOR_SYCL functions

The NVECTOR_SYCL module implementations of all vector operations listed in the sections in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VDotProdMulti`, `N_VWrmsNormVectorArray`, and `N_VWrmsNormMaskVectorArray` as support for arrays of reduction vectors is not yet supported. These function will be added to the NVECTOR_SYCL implementation in the future. The names of vector operations are obtained from those in the aforementioned sections by appending the suffix `_Sycl` (e.g., `N_VDestroy_Sycl`).

Additionally, the NVECTOR_SYCL module provides the following user-callable constructors for creating a new NVECTOR_SYCL:

`N_VNew_Sycl`

Prototype
```
N_Vector N_VNew_Sycl(sunindextype length, sycl::queue* Q)
```

Description This function creates and allocates memory for a SYCL `N_Vector`. The vector data array is allocated on both the host and device.

`N_VNewManaged_Sycl`

Prototype
```
N_Vector N_VNewManaged_Sycl(sunindextype length, sycl::queue* Q)
```

Description This function creates and allocates memory for a SYCL `N_Vector`. The vector data array is allocated in managed memory.

`N_VMake_Sycl`

Prototype
```
N_Vector N_VMake_Sycl(sunindextype length, realtype *h_data,
                      realtype *dev_data, sycl::queue* Q)
```

Description This function creates an NVECTOR_SYCL with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself.

`N_VMakeManaged_Sycl`

Prototype
```
N_Vector N_VMakeManaged_Sycl(sunindextype length, realtype *vdata,
                             sycl::queue* Q)
```

Description This function creates an NVECTOR_SYCL with a user-supplied managed memory data array. This function does not allocate memory for data itself.

N_VNewWithMemHelp_Sycl

Prototype `N_Vector N_VNewWithMemHelp_Sycl(sunindextype length, booleantype use_managed_mem, SUNMemoryHelper helper, sycl::queue* Q);`

Description This function creates an NVECTOR_SYCL which will use the `SUNMemoryHelper` object to allocate memory. If `use_managed_memory` is 0, then unmanaged memory is used, otherwise managed memory is used.

N_VNewEmpty_Sycl

Prototype `N_Vector N_VNewEmpty_Sycl()`

Description This function creates a new NVECTOR_SYCL where the members of the content structure have not been allocated. This utility function is used by the other constructors to create a new vector.

The following user-callable functions are provided for accessing the vector data arrays on the host and device and copying data between the two memory spaces. Note the generic NVECTOR operations `N_VGetArrayPointer()` and `N_VSetArrayPointer()` are mapped to the corresponding `HostArray` functions given below. To ensure memory coherency, a user will need to call the `CopyTo` or `CopyFrom` functions as necessary to transfer data between the host and device, unless managed (shared) memory is used.

N_VGetHostArrayPointer_Sycl

Prototype `realtype *N_VGetHostArrayPointer_Sycl(N_Vector v)`

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

N_VGetDeviceArrayPointer_Sycl

Prototype `realtype *N_VGetDeviceArrayPointer_Sycl(N_Vector v)`

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

N_VSetHostArrayPointer_Sycl

Prototype `realtype *N_VSetHostArrayPointer_Sycl(N_Vector v)`

Description This function sets the pointer to the vector data on the host. The existing pointer *will not* be freed first.

N_VSetDeviceArrayPointer_Sycl

Prototype `realtype *N_VSetDeviceArrayPointer_Sycl(N_Vector v)`

Description This function sets pointer to the vector data on the device. The existing pointer *will not* be freed first.

N_VCopyToDevice_Sycl

Prototype `realtype *N_VCopyToDevice_Sycl(N_Vector v)`

Description This function copies host vector data to the device.

N_VCopyFromDevice_Sycl

Prototype `realtype *N_VCopyFromDevice_Sycl(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VIsManagedMemory_Sycl`

Prototype `booleantype *N_VIsManagedMemory_Sycl(N_Vector v)`

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

The following user-callable function is provided to set the execution policies for how SYCL kernels are launched on a device.

`N_VSetKernelExecPolicy_Sycl`

Prototype
```
int N_VSetKernelExecPolicy_Sycl(N_Vector v,
                                SUNSyclExecPolicy *stream_exec_policy,
                                SUNSyclExecPolicy *reduce_exec_policy)
```

Description This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction kernels. By default the vector is setup to use the `SUNSyclThreadDirectExecPolicy` and `SUNSyclBlockReduceExecPolicy`. See Section 7.12.2 below for more information about the `SUNSyclExecPolicy` class.

Note: All vectors used in a single instance of a SUNDIALS package must use the same execution policy. It is **strongly recommended** that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors.

The following user-callable functions are provided to print the host vector data array. Unless managed memory is used, a user may need to call `N_VCopyFromDevice_Sycl()` to ensure consistency between the host and device array.

`N_VPrint_Sycl`

Prototype `void N_VPrint_Sycl(N_Vector v)`

Description This function prints the host data of a SYCL vector to `stdout`.

`N_VPrintFile_Sycl`

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

Description This function prints the host data of a SYCL vector to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_SYCL 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 one of the above constructors, enable/disable the desired operations on that vector with the functions below, and then use this vector in conjunction `N_VClone` to create any additional vectors. 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 by any of the above constructors will have the default settings for the NVECTOR_SYCL module.

`N_VEnableFusedOps_Sycl`

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

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

`N_VEnableLinearCombination_Sycl`

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

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

`N_VEnableScaleAddMulti_Sycl`

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

`N_VEnableLinearSumVectorArray_Sycl`

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

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

`N_VEnableScaleVectorArray_Sycl`

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

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

`N_VEnableConstVectorArray_Sycl`

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

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

`N_VEnableScaleAddMultiVectorArray_Sycl`

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

`N_VEnableLinearCombinationVectorArray_Sycl`

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

Description This function enables (`SUNTRUE`) or disables (`SUNFALSE`) the linear combination operation for vector arrays in the SYCL 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_Sycl`, `v`, it is recommended to use `N_VGetDeviceArrayPointer` to access the device array or `N_VGetArrayPointer` for the host array. When using managed (shared) memory, either function may be used. To ensure memory coherency, a user may need to call the `CopyTo` or `CopyFrom` functions as necessary to transfer data between the host and device, unless managed (shared) memory is used.

- To maximize efficiency, vector operations in the NVECTOR_SYCL implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.12.2 The SUNSyclExecPolicy Class

In order to provide maximum flexibility to users, the SYCL kernel execution parameters used by kernels within SUNDIALS are defined by objects of the `sundials::SyclExecPolicy` abstract class type (this class can be accessed in the global namespace as `SUNSyclExecPolicy`). Thus, users may provide custom execution policies that fit the needs of their problem. The `sundials::SyclExecPolicy` is defined in the header file `sundials_sycl_policies.hpp`, as follows:

```
class SyclExecPolicy
{
public:
   virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
   virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
   virtual SyclExecPolicy* clone() const = 0;
   virtual ~SyclExecPolicy() {}
};
```

For consistency the function names and behavior mirror the execution policies for the CUDA and HIP vectors. In the SYCL case the `blockSize` is the local work-group range in a one-dimensional `nd_range` (threads per group). The `gridSize` is the number of local work groups so the global work-group range in a one-dimensional `nd_range` is `blockSize * gridSize` (total number of threads). All vector kernels are written with a many-to-one mapping where work units (vector elements) are mapped in a round-robin manner across the global range. As such, the `blockSize` and `gridSize` can be set to any positive value.

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided `sundials::SyclThreadDirectExecPolicy` (aka in the global namespace as `SUNSyclThreadDirectExecPolicy`) class is a good example of a what a custom execution policy may look like:

```
class SyclThreadDirectExecPolicy : public SyclExecPolicy
{
public:
   SyclThreadDirectExecPolicy(const size_t blockDim)
      : blockDim_(blockDim)
   {}

   SyclThreadDirectExecPolicy(const SyclThreadDirectExecPolicy& ex)
      : blockDim_(ex.blockDim_)
   {}

   virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const
   {
```

```
      return (numWorkUnits + blockSize() - 1) / blockSize();
   }

   virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const
   {
      return blockDim_;
   }

   virtual SyclExecPolicy* clone() const
   {
      return static_cast<SyclExecPolicy*>(new SyclThreadDirectExecPolicy(*this));
   }

private:
   const size_t blockDim_;
};
```

SUNDIALS provides the following execution policies:

1. `SUNSyclThreadDirectExecPolicy(const size_t blockDim)` is for kernels performing streaming operations and maps each work unit (vector element) to a work-item (thread). Based on the local work-group range (number of threads per group, `blockSize`) the number of local work-groups (`gridSize`) is computed so there are enough work-items in the global work-group range (total number of threads, `blockSize * gridSize`) for one work unit per work-item (thread).

2. `SUNSyclGridStrideExecPolicy(const size_t blockDim, const size_t gridDim)` is for kernels performing streaming operations and maps each work unit (vector element) to a work-item (thread) in a round-robin manner so the local work-group range (number of threads per group, `blockSize`) and the number of local work-groups (`gridSize`) can be set to any positive value. In this case the global work-group range (total number of threads, `blockSize * gridSize`) may be less than the number of work units (vector elements).

3. `SUNSyclBlockReduceExecPolicy(const size_t blockDim)` is for kernels performing a reduction, the local work-group range (number of threads per group, `blockSize`) and the number of local work-groups (`gridSize`) can be set to any positive value or the `gridSize` may be set to `0` in which case the global range is chosen so that there are enough threads for at most two work units per work-item.

By default the NVECTOR_SYCL module uses the `SUNSyclThreadDirectExecPolicy` and `SUNSyclBlockReduceExecPolicy` where the default `blockDim` is determined by querying the device for the `max_work_group_size`. User may specify different policies by constructing a new `SyclExecPolicy` and attaching it with `N_VSetKernelExecPolicy_Sycl()`. For example, a policy that uses 128 work-items (threads) per group can be created and attached like so:

```
N_Vector v = N_VNew_Sycl(length);
SUNSyclThreadDirectExecPolicy thread_direct(128);
SUNSyclBlockReduceExecPolicy  block_reduce(128);
flag = N_VSetKernelExecPolicy_Sycl(v, &thread_direct, &block_reduce);
```

These default policy objects can be reused for multiple SUNDIALS data structures (e.g. a `SUNMatrix` and an `N_Vector`) since they do not hold any modifiable state information.

7.13 The NVECTOR_OPENMPDEV implementation

In situations where a user has access to a device such as a GPU for offloading computation, SUNDIALS provides an NVECTOR implementation using OpenMP device offloading, called NVECTOR_OPENMPDEV.

The NVECTOR_OPENMPDEV implementation defines the *content* field of the `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array on the host, a pointer to the beginning of a contiguous data array on the device, and a boolean flag `own_data` which specifies the ownership of host and device data arrays.

```
struct _N_VectorContent_OpenMPDEV {
  sunindextype length;
  booleantype own_data;
  realtype *host_data;
  realtype *dev_data;
};
```

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

7.13.1 NVECTOR_OPENMPDEV accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMPDEV vector.

- `NV_CONTENT_OMPDEV`

  This routine gives access to the contents of the NVECTOR_OPENMPDEV vector `N_Vector`.

  The assignment `v_cont = NV_CONTENT_OMPDEV(v)` sets `v_cont` to be a pointer to the NVECTOR_OPENMPDEV `N_Vector` content structure.

  Implementation:

  ```
  #define NV_CONTENT_OMPDEV(v) ( (N_VectorContent_OpenMPDEV)(v->content) )
  ```

- `NV_OWN_DATA_OMPDEV`, `NV_DATA_HOST_OMPDEV`, `NV_DATA_DEV_OMPDEV`, `NV_LENGTH_OMPDEV`

  These macros give individual access to the parts of the content of an NVECTOR_OPENMPDEV `N_Vector`.

  The assignment `v_data = NV_DATA_HOST_OMPDEV(v)` sets `v_data` to be a pointer to the first component of the data on the host for the `N_Vector v`. The assignment `NV_DATA_HOST_OMPDEV(v) = v_data` sets the host component array of `v` to be `v_data` by storing the pointer `v_data`.

  The assignment `v_dev_data = NV_DATA_DEV_OMPDEV(v)` sets `v_dev_data` to be a pointer to the first component of the data on the device for the `N_Vector v`. The assignment `NV_DATA_DEV_OMPDEV(v) = v_dev_data` sets the device component array of `v` to be `v_dev_data` by storing the pointer `v_dev_data`.

  The assignment `v_len = NV_LENGTH_OMPDEV(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_OMPDEV(v) = len_v` sets the length of `v` to be `len_v`.

  Implementation:

  ```
  #define NV_OWN_DATA_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->own_data )
  #define NV_DATA_HOST_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->host_data )
  #define NV_DATA_DEV_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->dev_data )
  #define NV_LENGTH_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->length )
  ```

7.13.2 NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. It also provides methods for copying from the host to the device and vice versa.

The names of vector operations are obtained from those in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix _OpenMPDEV (e.g. N_VDestroy_OpenMPDEV). The module NVECTOR_OPENMPDEV provides the following additional user-callable routines:

N_VNew_OpenMPDEV

Prototype `N_Vector N_VNew_OpenMPDEV(sunindextype vec_length)`

Description This function creates and allocates memory for an NVECTOR_OPENMPDEV `N_Vector`.

N_VNewEmpty_OpenMPDEV

Prototype `N_Vector N_VNewEmpty_OpenMPDEV(sunindextype vec_length)`

Description This function creates a new NVECTOR_OPENMPDEV `N_Vector` with an empty (`NULL`) host and device data arrays.

N_VMake_OpenMPDEV

Prototype
```
N_Vector N_VMake_OpenMPDEV(sunindextype vec_length, realtype *h_vdata,
                           realtype *d_vdata)
```

Description This function creates an NVECTOR_OPENMPDEV vector with user-supplied vector data arrays `h_vdata` and `d_vdata`. This function does not allocate memory for data itself.

N_VCloneVectorArray_OpenMPDEV

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

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

N_VCloneVectorArrayEmpty_OpenMPDEV

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

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

N_VDestroyVectorArray_OpenMPDEV

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

Description This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_OpenMPDEV` or with `N_VCloneVectorArrayEmpty_OpenMPDEV`.

N_VGetHostArrayPointer_OpenMPDEV

Prototype `realtype *N_VGetHostArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the host data array.

N_VGetDeviceArrayPointer_OpenMPDEV

Prototype `realtype *N_VGetDeviceArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the device data array.

`N_VPrint_OpenMPDEV`

Prototype `void N_VPrint_OpenMPDEV(N_Vector v)`

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

`N_VPrintFile_OpenMPDEV`

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

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

`N_VCopyToDevice_OpenMPDEV`

Prototype `void N_VCopyToDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's host data array to the device data array.

`N_VCopyFromDevice_OpenMPDEV`

Prototype `void N_VCopyFromDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's device data array to the host data array.

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

`N_VEnableFusedOps_OpenMPDEV`

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

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

`N_VEnableLinearCombination_OpenMPDEV`

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

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

`N_VEnableScaleAddMulti_OpenMPDEV`

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

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

`N_VEnableDotProdMulti_OpenMPDEV`

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

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

`N_VEnableLinearSumVectorArray_OpenMPDEV`

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

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

`N_VEnableScaleVectorArray_OpenMPDEV`

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

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

`N_VEnableConstVectorArray_OpenMPDEV`

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

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

`N_VEnableWrmsNormVectorArray_OpenMPDEV`

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

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

`N_VEnableWrmsNormMaskVectorArray_OpenMPDEV`

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

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

`N_VEnableScaleAddMultiVectorArray_OpenMPDEV`

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

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

`N_VEnableLinearCombinationVectorArray_OpenMPDEV`

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

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

Notes

- When looping over the components of an `N_Vector v`, it is most efficient to first obtain the component array via `h_data = NV_DATA_HOST_OMPDEV(v)` for the host array or `d_data = NV_DATA_DEV_OMPDEV(v)` for the device array and then access `h_data[i]` or `d_data[i]` within the loop.

- When accessing individual components of an `N_Vector v` on the host remember to first copy the array back from the device with `N_VCopyFromDevice_OpenMPDEV(v)` to ensure the array is up to date.

- `N_VNewEmpty_OpenMPDEV`, `N_VMake_OpenMPDEV`, and `N_VCloneVectorArrayEmpty_OpenMPDEV` set the field `own_data` = `SUNFALSE`. `N_VDestroy_OpenMPDEV` and `N_VDestroyVectorArray_OpenMPDEV` will not attempt to free the pointer *data* for any `N_Vector` with `own_data` set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the *data* pointer.

- To maximize efficiency, vector operations in the NVECTOR_OPENMPDEV implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.

7.14 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, int, sunindextype> vector_type;
```

The Tpetra vector will use the SUNDIALS-specified `realtype` as its scalar type, `int` as its local ordinal type, and `sunindextype` as the global ordinal type. 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.

7.14.1 NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in Tables 7.1.1, 7.1.4, and 7.1.4, 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 [34].

The names of vector operations are obtained from those in Tables 7.1.1, 7.1.4, and 7.1.4 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.

7.15 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 within a computational node. 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 two generic use cases for this implementation:

A. *Heterogeneous computational architectures*: 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 serial component based on NVECTOR_SERIAL, another component for GPU accelerators based on NVECTOR_CUDA, and another threaded component based on NVECTOR_OPENMP.

B. *Structure of arrays (SOA) data layouts*: 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 implementation 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. 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.

7.15.1 NVECTOR_MANYVECTOR structure

The NVECTOR_MANYVECTOR implementation defines the *content* field of `N_Vector` to be a structure containing the number of subvectors comprising the ManyVector, the global length of the ManyVector (including all subvectors), 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 {
  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.

7.15.2 NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VGetArrayPointer`, `N_VSetArrayPointer`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. As such, this vector cannot be used with the SUNDIALS Fortran-77 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 7.1.1, 7.1.2, 7.1.3, and 7.1.4 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.

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., a memory allocation failure occurred).

Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions `N_VNewVectorArray`, and `N_VSetVecAtIndexVectorArray` to create the `N_Vector*` argument. This is further explained in Chapter 5.1.3.5, and the functions are documented in Chapter 7.1.6.

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

`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.

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

`N_VGetSubvectorArrayPointer_ManyVector`

Prototype `realtype *N_VGetSubvectorArrayPointer_ManyVector(N_Vector v, sunindextype vec_num);`

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

If the input `vec_num` is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then `NULL` is returned.

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

`N_VSetSubvectorArrayPointer_ManyVector`

Prototype `int N_VSetSubvectorArrayPointer_ManyVector(realtype *v_data, N_Vector v, sunindextype vec_num);`

Description This function sets the data array pointer for the `vec_num` subvector from the NVECTOR array.

If the input `vec_num` is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then this routine returns `-1`; otherwise it returns `0`.

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

`N_VGetNumSubvectors_ManyVector`

Prototype `sunindextype N_VGetNumSubvectors_ManyVector(N_Vector v);`

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

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

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`, 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` 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`.

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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`.

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

`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 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`.

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

Notes

- `N_VNew_ManyVector` sets 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 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 subvector representations.

7.16 The NVECTOR_MPIMANYVECTOR implementation

The NVECTOR_MPIMANYVECTOR implementation of the NVECTOR module provided with SUNDIALS is designed to facilitate problems with an inherent data partitioning for the solution vector, and when using distributed-memory parallel architectures. As such, the MPIManyVector implementation supports all use cases allowed by the MPI-unaware ManyVector implementation, as well as partitioning data between nodes in a parallel environment. 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_MPIMANYVECTOR. We envision three generic use cases for this implementation:

A. *Heterogeneous computational architectures (single-node or multi-node)*: 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 (multi-node)*: 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 (single-node or multi-node)*: 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_MPIMANYVECTOR for the overall "solution".

We note that the above use cases are not mutually exclusive, and the NVECTOR_MPIMANYVECTOR implementation should support arbitrary combinations of these cases.

The NVECTOR_MPIMANYVECTOR 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 7.1.4.

Additionally, NVECTOR_MPIMANYVECTOR 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_MPIMANYVECTOR. 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.

7.16.1 NVECTOR_MPIMANYVECTOR structure

The NVECTOR_MPIMANYVECTOR implementation defines the *content* field of `N_Vector` to be a structure containing the MPI communicator (or `MPI_COMM_NULL` if running on a single-node), the number of subvectors comprising the MPIManyVector, the global length of the MPIManyVector (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_MPIManyVector {
  MPI_Comm      comm;            /* overall MPI communicator        */
  sunindextype  num_subvectors;  /* number of vectors attached      */
  sunindextype  global_length;   /* overall mpimanyvector 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_mpimanyvector.h`. The installed module library to link against is `libsundials_nvecmpimanyvector.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

Note: If SUNDIALS is configured with MPI disabled, then the MPIManyVector library will not be built. Furthermore, any user codes that include `nvector_mpimanyvector.h` *must* be compiled using an MPI-aware compiler (whether the specific user code utilizes MPI or not). We note that the NVECTOR_MANYVECTOR implementation is designed for ManyVector use cases in an MPI-unaware environment.

7.16.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, except for `N_VGetArrayPointer`, `N_VSetArrayPointer`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. As such, this vector cannot be used with the SUNDIALS Fortran-77 interfaces, nor with the SUNDIALS direct solvers and preconditioners. Instead, the NVECTOR_MPIMANYVECTOR 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 7.1.1, 7.1.2, 7.1.3, and 7.1.4 by appending the suffix `_MPIManyVector` (e.g. `N_VDestroy_MPIManyVector`). The module NVECTOR_MPIMANYVECTOR provides the following additional user-callable routines:

`N_VNew_MPIManyVector`

Prototype
```
N_Vector N_VNew_MPIManyVector(sunindextype num_subvectors,
                              N_Vector *vec_array);
```

Description This function creates an MPIManyVector 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 MPIManyVector that contains them.

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

Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions `N_VNewVectorArray`, and `N_VSetVecAtIndexVectorArray` to create the `N_Vector*` argument. This is further explained in Chapter 5.1.3.5, and the functions are documented in Chapter 7.1.6.

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

`N_VMake_MPIManyVector`

Prototype `N_Vector N_VMake_MPIManyVector(MPI_Comm comm, sunindextype num_subvectors, N_Vector *vec_array);`

Description This function creates an MPIManyVector 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 this user-created MPI communicator. 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_MPIManyVector`.

If all subvectors are MPI-unaware, then the input `comm` argument should be `MPI_COMM_NULL`, although in this case, it would be simpler to call `N_VNew_MPIManyVector` instead, or to just use the NVECTOR_MANYVECTOR module.

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 MPIManyVector that contains them.

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

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

`N_VGetSubvector_MPIManyVector`

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

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

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

`N_VGetSubvectorArrayPointer_MPIManyVector`

Prototype `realtype *N_VGetSubvectorArrayPointer_MPIManyVector(N_Vector v, sunindextype vec_num);`

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

If the input `vec_num` is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then `NULL` is returned.

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

`N_VSetSubvectorArrayPointer_MPIManyVector`

Prototype `int N_VSetSubvectorArrayPointer_MPIManyVector(realtype *v_data, N_Vector v, sunindextype vec_num);`

Description This function sets the data array pointer for the `vec_num` subvector from the NVECTOR array.

If the input `vec_num` is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then this routine returns `-1`; otherwise it returns `0`.

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

`N_VGetNumSubvectors_MPIManyVector`

Prototype `sunindextype N_VGetNumSubvectors_MPIManyVector(N_Vector v);`

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

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

By default all fused and vector array operations are disabled in the NVECTOR_MPIMANYVECTOR 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_MPIManyVector` or `N_VMake_MPIManyVector`, 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_MPIManyVector` and `N_VMake_MPIManyVector` will have the default settings for the NVECTOR_MPIMANYVECTOR 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 MPIManyVector in `N_VNew_MPIManyVector` or `N_VMake_MPIManyVector`.

`N_VEnableFusedOps_MPIManyVector`

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

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

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

`N_VEnableLinearCombination_MPIManyVector`

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

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

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

`N_VEnableScaleAddMulti_MPIManyVector`

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

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

`N_VEnableDotProdMulti_MPIManyVector`

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

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

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

`N_VEnableLinearSumVectorArray_MPIManyVector`

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

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

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

`N_VEnableScaleVectorArray_MPIManyVector`

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

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

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

`N_VEnableConstVectorArray_MPIManyVector`

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

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

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

`N_VEnableWrmsNormVectorArray_MPIManyVector`

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

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

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

`N_VEnableWrmsNormMaskVectorArray_MPIManyVector`

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

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

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

Notes

- `N_VNew_MPIManyVector` and `N_VMake_MPIManyVector` set the field *own_data* = `SUNFALSE`. `N_VDestroy_MPIManyVector` 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_MPIMANYVECTOR 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 subvector representations.

7.17 The NVECTOR_MPIPLUSX implementation

The NVECTOR_MPIPLUSX implementation of the NVECTOR module provided with SUNDIALS is designed to facilitate the MPI+X paradigm, where X is some form of on-node (local) parallelism (e.g. OpenMP, CUDA). This paradigm is becoming increasingly popular with the rise of heterogeneous computing architectures.

The NVECTOR_MPIPLUSX implementation is designed to work with any NVECTOR that implements the minimum *required* set of operations. However, it is not recommended to use the NVECTOR_PARALLEL, NVECTOR_PARHYP, NVECTOR_PETSC, or NVECTOR_TRILINOS implementations underneath the NVECTOR_MPIPLUSX module since they already provide MPI capabilities.

7.17.1 NVECTOR_MPIPLUSX structure

The NVECTOR_MPIPLUSX implementation is a thin wrapper around the NVECTOR_MPIMANYVECTOR. Accordingly, it adopts the same content structure as defined in Section 7.16.1.

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

Note: If SUNDIALS is configured with MPI disabled, then the mpiplusx library will not be built. Furthermore, any user codes that include `nvector_mpiplusx.h` *must* be compiled using an MPI-aware compiler.

7.17.2 NVECTOR_MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in Tables 7.1.1, 7.1.2, 7.1.3, and 7.1.4, from the NVECTOR_MPIMANYVECTOR (see section 7.16.2) except for `N_VGetArrayPointer` and `N_VSetArrayPointer`; the module provides its own implementation of these functions that call the local vector implementations. Therefore, the NVECTOR_MPIPLUSX module implements all of the operations listed in the referenced sections except for `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. Accordingly, it's compatibility with the SUNDIALS Fortran-77 interface, and with the SUNDIALS direct solvers and preconditioners depends on the local vector implementation.

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

`N_VMake_MPIPlusX`

Prototype
```
N_Vector N_VMake_MPIPlusX(MPI_Comm comm,
                          N_Vector *local_vector);
```

Description This function creates an MPIPlusX vector from an existing local (i.e. on-node) NVECTOR object, and a user-created MPI communicator.

The input `comm` should be this user-created MPI communicator. 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_MPIPlusX`.

This routine will copy the N_Vector pointer to the input local_vector, so the underlying local NVECTOR object should not be destroyed before the mpiplusx that contains it.

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

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

N_VGetLocalVector_MPIPlusX

Prototype `N_Vector N_VGetLocalVector_MPIPlusX(N_Vector v);`

Description This function returns the local vector underneath the the MPIPlusX NVECTOR.

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

N_VGetArrayPointer_MPIPlusX

Prototype `realtype* N_VGetLocalVector_MPIPlusX(N_Vector v);`

Description This function returns the data array pointer for the local vector if the local vector implements the N_VGetArrayPointer operation; otherwise it returns NULL.

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

N_VSetArrayPointer_MPIPlusX

Prototype `void N_VSetArrayPointer_MPIPlusX(realtype *data, N_Vector v);`

Description This function sets the data array pointer for the local vector if the local vector implements the N_VSetArrayPointer operation.

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

The NVECTOR_MPIPLUSX module does not implement any fused or vector array operations. Instead users should enable/disable fused operations on the local vector.

Notes

- N_VMake_MPIPlusX sets the field *own_data* = SUNFALSE.
  and N_VDestroy_MPIPlusX will not call N_VDestroy on the local vector. In this case, it is the user's responsibility to deallocate the local vector.

- To maximize efficiency, arithmetic vector operations in the NVECTOR_MPIPLUSX 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 local vector representations.

7.18 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 8

Description of the SUNMatrix module

For problems that involve direct methods for solving linear systems, the SUNDIALS solvers not only operate on generic vectors, but also on generic matrices (of type `SUNMatrix`), through a set of operations defined by the particular SUNMATRIX implementation. Users can provide their own specific implementation of the SUNMATRIX module, particularly in cases where they provide their own NVECTOR and/or linear solver modules, and require matrices that are compatible with those implementations. Alternately, we provide three SUNMATRIX implementations: dense, banded, and sparse. The generic operations are described below, and descriptions of the implementations provided with SUNDIALS follow.

8.1 The SUNMatrix API

The SUNMATRIX API can be grouped into two sets of functions: the core matrix operations, and utility functions. Section 8.1.1 lists the core operations, while Section 8.1.2 lists the utility functions.

8.1.1 SUNMatrix core functions

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

`SUNMatGetID`

Call `id = SUNMatGetID(A);`

Description 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.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object

Return value A `SUNMATRIX_ID`, possible values are given in the Table 8.2.

F2003 Name `FSUNMatGetID`

`SUNMatClone`

Call `B = SUNMatClone(A);`

Description 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.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object

Return value `SUNMatrix`

F2003 Name `FSUNMatClone`

F2003 Call
```
type(SUNMatrix), pointer ::  B
B => FSUNMatClone(A)
```

`SUNMatDestroy`

Call `SUNMatDestroy(A);`

Description Destroys `A` and frees memory allocated for its internal data.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object

Return value None

F2003 Name `FSUNMatDestroy`

`SUNMatSpace`

Call `ier = SUNMatSpace(A, &lrw, &liw);`

Description 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.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object
`lrw` (`sunindextype*`) the number of realtype words
`liw` (`sunindextype*`) the number of integer words

Return value None

Notes 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.

F2003 Name `FSUNMatSpace`

F2003 Call
```
integer(c_long) ::  lrw(1), liw(1)
ier = FSUNMatSpace(A, lrw, liw)
```

`SUNMatZero`

Call `ier = SUNMatZero(A);`

Description Performs the operation $A_{ij} = 0$ for all entries of the matrix A.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatZero`

`SUNMatCopy`

Call `ier = SUNMatCopy(A,B);`

Description Performs the operation $B_{ij} = A_{i,j}$ for all entries of the matrices A and B.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object
`B` (`SUNMatrix`) a SUNMATRIX object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatCopy`

`SUNMatScaleAdd`

Call `ier = SUNMatScaleAdd(c, A, B);`

Description Performs the operation $A = cA + B$.

Arguments `c` (`realtype`) constant that scales `A`
`A` (`SUNMatrix`) a SUNMATRIX object
`B` (`SUNMatrix`) a SUNMATRIX object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatScaleAdd`

`SUNMatScaleAddI`

Call `ier = SUNMatScaleAddI(c, A);`

Description Performs the operation $A = cA + I$.

Arguments `c` (`realtype`) constant that scales `A`
`A` (`SUNMatrix`) a SUNMATRIX object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatScaleAddI`

`SUNMatMatvecSetup`

Call `ier = SUNMatMatvecSetup(A);`

Description Performs any setup necessary to perform a matrix-vector product. It is useful for SUNMatrix implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatMatvecSetup`

`SUNMatMatvec`

Call `ier = SUNMatMatvec(A, x, y);`

Description 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.

Arguments `A` (`SUNMatrix`) a SUNMATRIX object
`x` (`N_Vector`) a NVECTOR object
y (`N_Vector`) an output NVECTOR object

Return value A SUNMATRIX return code of type `int` denoting success/failure

F2003 Name `FSUNMatMatvec`

8.1.2 SUNMatrix utility functions

To aid in the creation of custom SUNMATRIX modules the generic SUNMATRIX module provides two utility functions `SUNMatNewEmpty` and `SUNMatVCopyOps`.

`SUNMatNewEmpty`

Call `A = SUNMatNewEmpty();`

Description The function `SUNMatNewEmpty` allocates a new generic SUNMATRIX object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

Arguments None

Return value This function returns a `SUNMatrix` object. If an error occurs when allocating the object, then this routine will return `NULL`.

F2003 Name `FSUNMatNewEmpty`

`SUNMatFreeEmpty`

Call `SUNMatFreeEmpty(A);`

Description This routine frees the generic `SUNMatrix` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `A` (`SUNMatrix`) a `SUNMatrix` object

Return value None

F2003 Name `FSUNMatFreeEmpty`

`SUNMatCopyOps`

Call `retval = SUNMatCopyOps(A, B);`

Description The function `SUNMatCopyOps` copies the function pointers in the `ops` structure of `A` into the `ops` structure of `B`.

Arguments `A` (`SUNMatrix`) the matrix to copy operations from
`B` (`SUNMatrix`) the matrix to copy operations to

Return value This returns `0` if successful and a non-zero value if either of the inputs are `NULL` or the `ops` structure of either input is `NULL`.

F2003 Name `FSUNMatCopyOps`

8.1.3 SUNMatrix return codes

The functions provided to SUNMATRIX modules within the SUNDIALS-provided SUNMATRIX implementations utilize a common set of return codes, shown in Table 8.1. These adhere to a common pattern: 0 indicates success, and a negative value indicates a failure. The actual values of each return code are primarily to provide additional information to the user in case of a failure.

Table 8.1: Description of the `SUNMatrix` return codes

Name	Value	Description
SUNMAT_SUCCESS	0	successful call or converged solve

continued on next page

Table 8.2: 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_MAGMADENSE	Magma dense M × N matrix	2
SUNMATRIX_SPARSE	Sparse (CSR or CSC) M × N matrix	3
SUNMATRIX_SLUNRLOC	Adapter for the SuperLU_DIST SuperMatrix	4
SUNMATRIX_CUSPARSE	CUDA sparse CSR matrix	5
SUNMATRIX_CUSTOM	User-provided custom matrix	6

Name	Value	Description
SUNMAT_ILL_INPUT	-701	an illegal input has been provided to the function
SUNMAT_MEM_FAIL	-702	failed memory access or allocation
SUNMAT_OPERATION_FAIL	-703	a SUNMatrix operation returned nonzero
SUNMAT_MATVEC_SETUP_REQUIRED	-704	the SUNMatMatvecSetup routine needs to be called before calling SUNMatMatvec

8.1.4 SUNMatrix identifiers

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 8.2. It is recommended that a user-supplied SUNMATRIX implementation use the SUNMATRIX_CUSTOM identifier.

8.1.5 Compatibility of SUNMatrix modules

We note that not all SUNMATRIX types are compatible with all NVECTOR types provided with SUNDIALS. This is primarily due to the need for compatibility within the SUNMatMatvec routine; however, compatibility between SUNMATRIX and NVECTOR implementations is more crucial when considering their interaction within SUNLINSOL objects, as will be described in more detail in Chapter 9. More specifically, in Table 8.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 8.3: SUNDIALS matrix interfaces and vector implementations that can be used for each.

Matrix Interface	Serial	Parallel (MPI)	OpenMP	pThreads	*hypre* Vec.	PETSc Vec.	CUDA	RAJA	User Suppl.
Dense	✓		✓	✓					✓
Band	✓		✓	✓					✓
Sparse	✓		✓	✓					✓
SLUNRloc	✓	✓	✓	✓	✓	✓			✓
User supplied	✓	✓	✓	✓	✓	✓	✓	✓	✓

8.1.6 The generic SUNMatrix module implementation

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*);
};
```

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));
}
```

Section 8.1.1 contains a complete list of all matrix operations defined by the generic SUNMATRIX module.

The Fortran 2003 interface provides a bind(C) derived-type for the _generic_SUNMatrix and the _generic_SUNMatrix_Ops structures. Their definition is given below.

```
 type, bind(C), public :: SUNMatrix
  type(C_PTR), public :: content
  type(C_PTR), public :: ops
 end type SUNMatrix

 type, bind(C), public :: SUNMatrix_Ops
  type(C_FUNPTR), public :: getid
  type(C_FUNPTR), public :: clone
  type(C_FUNPTR), public :: destroy
  type(C_FUNPTR), public :: zero
  type(C_FUNPTR), public :: copy
  type(C_FUNPTR), public :: scaleadd
  type(C_FUNPTR), public :: scaleaddi
  type(C_FUNPTR), public :: matvecsetup
  type(C_FUNPTR), public :: matvec
  type(C_FUNPTR), public :: space
 end type SUNMatrix_Ops
```

8.1.7 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`.

It is recommended that a user-supplied SUNMATRIX implementation use the `SUNMATRIX_CUSTOM` identifier.

To aid in the creation of custom SUNMATRIX modules the generic SUNMATRIX module provides two utility functions `SUNMatNewEmpty` and `SUNMatVCopyOps`. When used in custom SUNMATRIX constructors and clone routines these functions will ease the introduction of any new optional matrix operations to the SUNMATRIX API by ensuring only required operations need to be set and all operations are copied when cloning a matrix. These functions are desrcribed in Section 8.1.2.

8.2 SUNMatrix functions used by IDA

In Table 8.4, 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 8.4: List of matrix functions usage by IDA code modules

	IDALS	IDABBDPRE
SUNMatGetID	✓	
SUNMatDestroy		✓
SUNMatZero	✓	✓
SUNMatSpace		†

The matrix functions listed in Section 8.1.1 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 Section 8.1.1 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.

8.3 The SUNMatrix_Dense implementation

The dense implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_DENSE, defines the *content* field of SUNMatrix to be the following structure:

```
struct _SUNMatrixContent_Dense {
  sunindextype M;
  sunindextype N;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

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

M - number of rows

N - number of columns

data - pointer to a contiguous block of realtype variables. The elements of the dense matrix are stored columnwise, i.e. the (i,j)-th element of a dense SUNMATRIX A (with $0 \le$ i $<$ M and $0 \le$ j $<$ N) may be accessed via data[j*M+i].

ldata - length of the data array (= M·N).

cols - array of pointers. cols[j] points to the first element of the j-th column of the matrix in the array data. The (i,j)-th element of a dense SUNMATRIX A (with $0 \le$ i $<$ M and $0 \le$ j $<$ N) may be accessed via cols[j][i].

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

8.3.1 SUNMatrix_Dense accessor macros

The following macros are provided to access the content of a SUNMATRIX_DENSE matrix. The prefix SM_ in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix _D denotes that these are specific to the *dense* version.

- SM_CONTENT_D

  This macro gives access to the contents of the dense SUNMatrix.

  The assignment A_cont = SM_CONTENT_D(A) sets A_cont to be a pointer to the dense SUNMatrix content structure.

  Implementation:

  ```
  #define SM_CONTENT_D(A)     ( (SUNMatrixContent_Dense)(A->content) )
  ```

- SM_ROWS_D, SM_COLUMNS_D, and SM_LDATA_D

  These macros give individual access to various lengths relevant to the content of a dense SUNMatrix.

  These may be used either to retrieve or to set these values. For example, the assignment A_rows = SM_ROWS_D(A) sets A_rows to be the number of rows in the matrix A. Similarly, the assignment SM_COLUMNS_D(A) = A_cols sets the number of columns in A to equal A_cols.

  Implementation:

  ```
  #define SM_ROWS_D(A)        ( SM_CONTENT_D(A)->M )
  ```

```
#define SM_COLUMNS_D(A)     ( SM_CONTENT_D(A)->N )
#define SM_LDATA_D(A)       ( SM_CONTENT_D(A)->ldata )
```

- SM_DATA_D and SM_COLS_D

  These macros give access to the data and cols pointers for the matrix entries.

  The assignment A_data = SM_DATA_D(A) sets A_data to be a pointer to the first component of the data array for the dense SUNMatrix A. The assignment SM_DATA_D(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_cols = SM_COLS_D(A) sets A_cols to be a pointer to the array of column pointers for the dense SUNMatrix A. The assignment SM_COLS_D(A) = A_cols sets the column pointer array of A to be A_cols by storing the pointer A_cols.

  Implementation:

```
#define SM_DATA_D(A)        ( SM_CONTENT_D(A)->data )
#define SM_COLS_D(A)        ( SM_CONTENT_D(A)->cols )
```

- SM_COLUMN_D and SM_ELEMENT_D

  These macros give access to the individual columns and entries of the data array of a dense SUNMatrix.

  The assignment col_j = SM_COLUMN_D(A,j) sets col_j to be a pointer to the first entry of the j-th column of the M × N dense matrix A (with $0 \le$ j $<$ N). The type of the expression SM_COLUMN_D(A,j) is realtype *. The pointer returned by the call SM_COLUMN_D(A,j) can be treated as an array which is indexed from 0 to M − 1.

  The assignments SM_ELEMENT_D(A,i,j) = a_ij and a_ij = SM_ELEMENT_D(A,i,j) reference the (i,j)-th element of the M × N dense matrix A (with $0 \le$ i $<$ M and $0 \le$ j $<$ N).

  Implementation:

```
#define SM_COLUMN_D(A,j)    ( (SM_CONTENT_D(A)->cols)[j] )
#define SM_ELEMENT_D(A,i,j) ( (SM_CONTENT_D(A)->cols)[j][i] )
```

8.3.2 SUNMatrix_Dense functions

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Section 8.1.1. Their names are obtained from those in Section 8.1.1 by appending the suffix _Dense (e.g. SUNMatCopy_Dense). All the standard matrix operations listed in Section 8.1.1 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.

8.3.3 SUNMatrix_Dense Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the SUNMATRIX_DENSE module also includes the FORTRAN-callable function `FSUNDenseMatInit(code, M, N, ier)` to initialize this SUNMATRIX_DENSE module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `M` and `N` are the corresponding dense matrix construction arguments (declared to match C type `long int`); and `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. Additionally, when using ARKODE with a non-identity mass matrix, the FORTRAN-callable function `FSUNDenseMassMatInit(M, N, ier)` initializes this SUNMATRIX_DENSE module for storing the mass matrix.

8.4 The SUNMatrix_Band implementation

The banded implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_BAND, defines the *content* field of `SUNMatrix` to be the following structure:

```
struct _SUNMatrixContent_Band {
  sunindextype M;
  sunindextype N;
  sunindextype mu;
  sunindextype ml;
  sunindextype s_mu;
  sunindextype ldim;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

A diagram of the underlying data representation in a banded matrix is shown in Figure 8.1. A more complete description of the parts of this *content* field is given below:

`M` - number of rows

`N` - number of columns (`N` = `M`)

`mu` - upper half-bandwidth, 0 ≤ `mu` < `N`

`ml` - lower half-bandwidth, 0 ≤ `ml` < `N`

`s_mu` - storage upper bandwidth, `mu` ≤ `s_mu` < `N`. The LU decomposition routines in the associated SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(`N`-1,`mu`+`ml`) because of partial pivoting. The `s_mu` field holds the upper half-bandwidth allocated for A.

`ldim` - leading dimension (`ldim` ≥ `s_mu`+`ml`+1)

`data` - pointer to a contiguous block of `realtype` variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. `data` is a pointer to `ldata` contiguous locations which hold the elements within the band of A.

`ldata` - length of the data array (= `ldim`·N)

`cols` - array of pointers. `cols[j]` is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from `s_mu`−`mu` (to access the uppermost element within the band in the j-th column) to `s_mu`+`ml` (to access the lowest element within the band in the j-th column). Indices from 0 to `s_mu`−`mu`−1 give access to extra storage elements required by the LU decomposition function. Finally, `cols[j][i-j+s_mu]` is the (i, j)-th element with j−`mu` ≤ i ≤ j+`ml`.

The header file to include when using this module is `sunmatrix/sunmatrix_band.h`. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixband` module library.

8.4.1 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 )
  ```

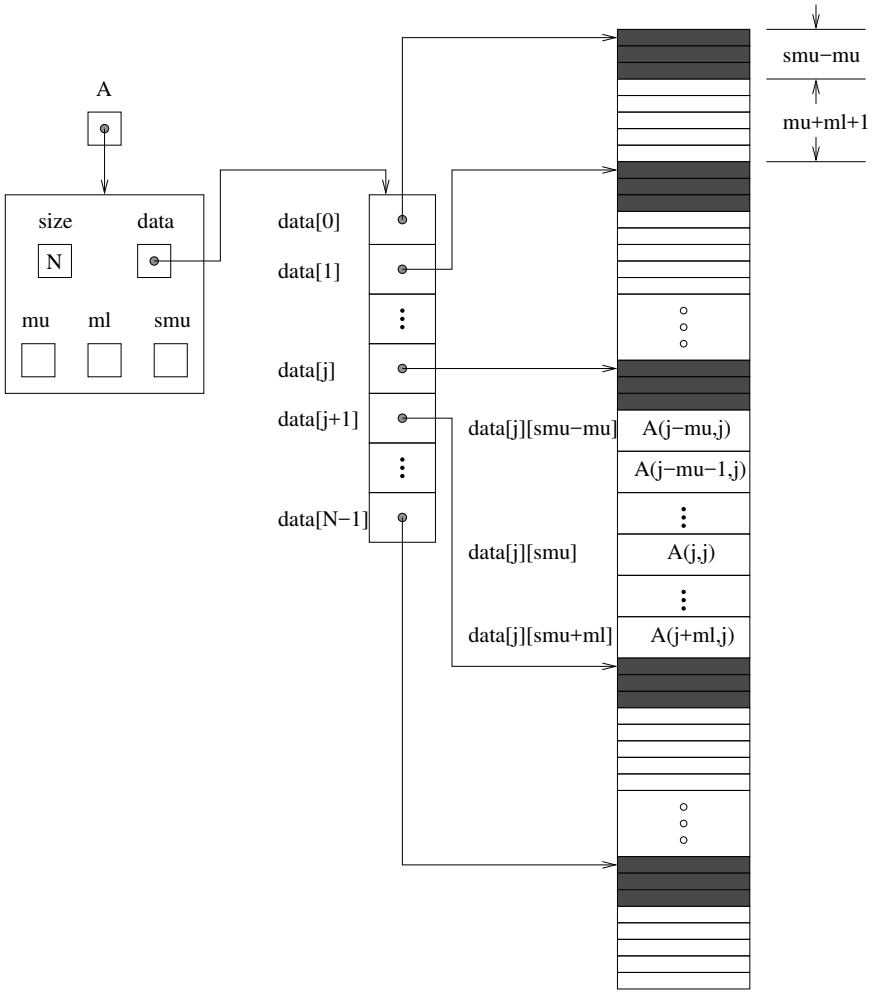

Figure 8.1: Diagram of the storage for the SUNMATRIX_BAND module. Here `A` is an `N` $\times$ `N` band matrix with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to `N` $- 1$ and the (i, j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the associated SUNLINSOL_BAND linear solver.

```
#define SM_SUBAND_B(A)      ( SM_CONTENT_B(A)->s_mu )
#define SM_LDIM_B(A)        ( SM_CONTENT_B(A)->ldim )
#define SM_LDATA_B(A)       ( SM_CONTENT_B(A)->ldata )
```

- SM_DATA_B and SM_COLS_B

  These macros give access to the data and cols pointers for the matrix entries.

  The assignment A_data = SM_DATA_B(A) sets A_data to be a pointer to the first component of the data array for the banded SUNMatrix A. The assignment SM_DATA_B(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_cols = SM_COLS_B(A) sets A_cols to be a pointer to the array of column pointers for the banded SUNMatrix A. The assignment SM_COLS_B(A) = A_cols sets the column pointer array of A to be A_cols by storing the pointer A_cols.

  Implementation:

```
#define SM_DATA_B(A)        ( SM_CONTENT_B(A)->data )
#define SM_COLS_B(A)        ( SM_CONTENT_B(A)->cols )
```

- SM_COLUMN_B, SM_COLUMN_ELEMENT_B, and SM_ELEMENT_B

  These macros give access to the individual columns and entries of the data array of a banded SUNMatrix.

  The assignments SM_ELEMENT_B(A,i,j) = a_ij and a_ij = SM_ELEMENT_B(A,i,j) reference the (i,j)-th element of the N × N band matrix A, where $0 \le$ i, j $\le$ N − 1. The location (i,j) should further satisfy j−mu $\le$ i $\le$ j+ml.

  The assignment col_j = SM_COLUMN_B(A,j) sets col_j to be a pointer to the diagonal element of the j-th column of the N × N band matrix A, $0 \le$ j $\le$ N − 1. The type of the expression SM_COLUMN_B(A,j) is realtype *. The pointer returned by the call SM_COLUMN_B(A,j) can be treated as an array which is indexed from −mu to ml.

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

  Implementation:

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

8.4.2 SUNMatrix_Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Section 8.1.1. Their names are obtained from those in Section 8.1.1 by appending the suffix _Band (e.g. SUNMatCopy_Band). All the standard matrix operations listed in Section 8.1.1 with the suffix _Band appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Band).

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

SUNBandMatrix

Prototype `SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu, sunindextype ml)`

Description This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, and the upper and lower half-bandwidths of the matrix, `mu` and `ml`. The stored upper bandwidth is set to `mu+ml` to accommodate subsequent factorization in the SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules.

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

`SUNBandMatrixStorage`

Prototype
```
SUNMatrix SUNBandMatrixStorage(sunindextype N, sunindextype mu,
                               sunindextype ml, sunindextype smu)
```

Description This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, the upper and lower half-bandwidths of the matrix, `mu` and `ml`, and the stored upper bandwidth, `smu`. When creating a band `SUNMatrix`, this value should be

- at least min(`N`-1,`mu`+`ml`) if the matrix will be used by the SUNLINSOL_BAND module;
- exactly equal to `mu`+`ml` if the matrix will be used by the SUNLINSOL_LAPACKBAND module;
- at least `mu` if used in some other manner.

Note: it is strongly recommended that users call the default constructor, `SUNBandMatrix`*, in all standard use cases. This advanced constructor is used internally within* SUNDIALS *solvers, and is provided to users who require banded matrices for non-default purposes.*

`SUNBandMatrix_Print`

Prototype
```
void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile)
```

Description This function prints the content of a banded `SUNMatrix` to the output stream specified by `outfile`. Note: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

`SUNBandMatrix_Rows`

Prototype
```
sunindextype SUNBandMatrix_Rows(SUNMatrix A)
```

Description This function returns the number of rows in the banded `SUNMatrix`.

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

`SUNBandMatrix_Columns`

Prototype
```
sunindextype SUNBandMatrix_Columns(SUNMatrix A)
```

Description This function returns the number of columns in the banded `SUNMatrix`.

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

`SUNBandMatrix_LowerBandwidth`

Prototype
```
sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A)
```

Description This function returns the lower half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_UpperBandwidth`

Prototype `sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A)`

Description This function returns the upper half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_StoredUpperBandwidth`

Prototype `sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A)`

Description This function returns the stored upper half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_LDim`

Prototype `sunindextype SUNBandMatrix_LDim(SUNMatrix A)`

Description This function returns the length of the leading dimension of the banded `SUNMatrix`.

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

`SUNBandMatrix_Data`

Prototype `realtype* SUNBandMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the banded `SUNMatrix`.

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

`SUNBandMatrix_Cols`

Prototype `realtype** SUNBandMatrix_Cols(SUNMatrix A)`

Description This function returns a pointer to the cols array for the banded `SUNMatrix`.

`SUNBandMatrix_Column`

Prototype `realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j)`

Description This function returns a pointer to the diagonal entry of the j-th column of the banded `SUNMatrix`. The resulting pointer should be indexed over the range $-$`mu` to `ml`.

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

Notes

- When looping over the components of a banded `SUNMatrix` `A`, the most efficient approaches are to:
  - First obtain the component array via `A_data = SM_DATA_B(A)` or `A_data = SUNBandMatrix_Data(A)` and then access `A_data[i]` within the loop.
  - First obtain the array of column pointers via `A_cols = SM_COLS_B(A)` or `A_cols = SUNBandMatrix_Cols(A)`, and then access `A_cols[j][i]` within the loop.
  - Within a loop over the columns, access the column pointer via `A_colj = SUNBandMatrix_Column(A,j)` and then to access the entries within that column using `SM_COLUMN_ELEMENT_B(A_colj,i,j)`.

All three of these are more efficient than using `SM_ELEMENT_B(A,i,j)` within a double loop.

- Within the `SUNMatMatvec_Band` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

8.4.3 SUNMatrix_Band Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the SUNMATRIX_BAND module also includes the FORTRAN-callable function `FSUNBandMatInit(code, N, mu, ml, ier)` to initialize this SUNMATRIX_BAND module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `N`, `mu`, and `ml` are the corresponding band matrix construction arguments (declared to match C type `long int`); and `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. Additionally, when using ARKODE with a non-identity mass matrix, the FORTRAN-callable function `FSUNBandMassMatInit(N, mu, ml, ier)` initializes this SUNMATRIX_BAND module for storing the mass matrix.

8.5 The SUNMatrix_Sparse implementation

The sparse implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_SPARSE, is designed to work with either *compressed-sparse-column* (CSC) or *compressed-sparse-row* (CSR) sparse matrix formats. To this end, it defines the *content* field of `SUNMatrix` to be the following structure:

```
struct _SUNMatrixContent_Sparse {
  sunindextype M;
  sunindextype N;
  sunindextype NNZ;
  sunindextype NP;
  realtype *data;
  int sparsetype;
  sunindextype *indexvals;
  sunindextype *indexptrs;
  /* CSC indices */
  sunindextype **rowvals;
```

```
  sunindextype **colptrs;
  /* CSR indices */
  sunindextype **colvals;
  sunindextype **rowptrs;
};
```

A diagram of the underlying data representation for a CSC matrix is shown in Figure 8.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

`M` - number of rows

`N` - number of columns

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

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

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

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

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

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

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

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

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

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

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

For example, the 5×4 CSC matrix

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

could be stored in this structure as either

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

or

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

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

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

```
M = 5;
N = 4;
NNZ = 8;
NP = M;
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 SUNMATRIX_SPARSE module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixsparse` module library.

8.5.1 SUNMatrix_Sparse accessor macros

The following macros are provided to access the content of a SUNMATRIX_SPARSE matrix. The prefix `SM_` in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix `_S` denotes that these are specific to the *sparse* version.

- `SM_CONTENT_S`

  This routine gives access to the contents of the sparse `SUNMatrix`.

  The assignment `A_cont = SM_CONTENT_S(A)` sets `A_cont` to be a pointer to the sparse `SUNMatrix` content structure.

  Implementation:

  ```
  #define SM_CONTENT_S(A)     ( (SUNMatrixContent_Sparse)(A->content) )
  ```

- `SM_ROWS_S`, `SM_COLUMNS_S`, `SM_NNZ_S`, `SM_NP_S`, and `SM_SPARSETYPE_S`

  These macros give individual access to various lengths relevant to the content of a sparse `SUNMatrix`.

  These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_S(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_S(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

  Implementation:

  ```
  #define SM_ROWS_S(A)        ( SM_CONTENT_S(A)->M )
  #define SM_COLUMNS_S(A)     ( SM_CONTENT_S(A)->N )
  #define SM_NNZ_S(A)         ( SM_CONTENT_S(A)->NNZ )
  #define SM_NP_S(A)          ( SM_CONTENT_S(A)->NP )
  #define SM_SPARSETYPE_S(A)  ( SM_CONTENT_S(A)->sparsetype )
  ```

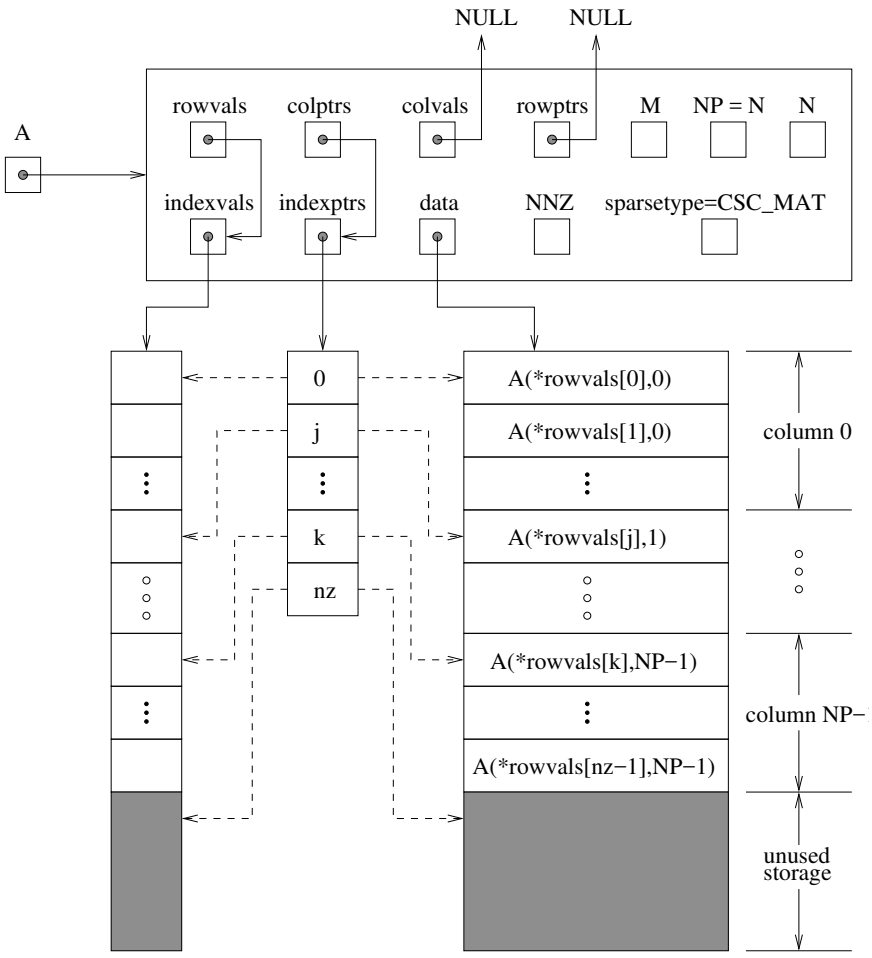

Figure 8.2: Diagram of the storage for a compressed-sparse-column matrix. Here `A` is an $\texttt{M} \times \texttt{N}$ sparse matrix with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to $\texttt{M} - 1$, corresponding to the row index (zero-based) of each nonzero value. The entries in `data` contain the values of the nonzero entries, with the row i, column j entry of `A` (again, zero-based) denoted as `A(i,j)`. The `indexptrs` array contains $\texttt{N}+1$ entries; the first `N` denote the starting index of each column within the `indexvals` and `data` arrays, while the final entry points one past the final nonzero entry. Here, although `NNZ` values are allocated, only `nz` are actually filled in; the greyed-out portions of `data` and `indexvals` indicate extra allocated space.

- SM_DATA_S, SM_INDEXVALS_S, and SM_INDEXPTRS_S

  These macros give access to the data and index arrays for the matrix entries.

  The assignment A_data = SM_DATA_S(A) sets A_data to be a pointer to the first component of the data array for the sparse SUNMatrix A. The assignment SM_DATA_S(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_indexvals = SM_INDEXVALS_S(A) sets A_indexvals to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix A. The assignment A_indexptrs = SM_INDEXPTRS_S(A) sets A_indexptrs to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).

  Implementation:

```
#define SM_DATA_S(A)        ( SM_CONTENT_S(A)->data )
#define SM_INDEXVALS_S(A)   ( SM_CONTENT_S(A)->indexvals )
#define SM_INDEXPTRS_S(A)   ( SM_CONTENT_S(A)->indexptrs )
```

8.5.2 SUNMatrix_Sparse functions

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Section 8.1.1. Their names are obtained from those in Section 8.1.1 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). All the standard matrix operations listed in Section 8.1.1 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, NVECTOR_PTHREADS, and NVECTOR_CUDA when using managed memory. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

8.5.3 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.

8.6 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 [8, 28, 40, 41]. It is designed to be used with the SUNLINSOL_SUPERLUDIST linear solver discussed in Section 9.10. 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.

8.6.1 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 SUNMatrix 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 SuperLU_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 Section 8.1.1:

- `SUNMatGetID_SLUNRloc` - returns `SUNMATRIX_SLUNRLOC`
- `SUNMatClone_SLUNRloc`
- `SUNMatDestroy_SLUNRloc`
- `SUNMatSpace_SLUNRloc` - this only returns information for the storage within the matrix interface, 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.

8.7 The SUNMatrix_cuSparse implementation

The SUNMATRIX_CUSPARSE implementation of the SUNMatrix module provided with SUNDIALS, is an interface to the NVIDIA cuSPARSE matrix for use on NVIDIA GPUs [7]. All data stored by this matrix implementation resides on the GPU at all times. The implementation currently supports the cuSPARSE CSR matrix format described in the cuSPARSE documentation as well as a unique low-storage format for block-diagonal matrices of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix}$$

where all the block matrices A_j share the same sparsity pattern. We will refer to this format as BCSR (not to be confused with the canonical BSR format where each block is stored as dense). In this format, the CSR column indices and row pointers are only stored for the first block and are computed only as necessary for other blocks. This can drastically reduce the amount of storage required compared to the regular CSR format when there is a large number of blocks. This format is well-suited for, and intended to be used with the SUNLinearSolver_cuSolverSp_batchQR linear solver (see Section 9.12).

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

The SUNMatrix_cuSparse module is experimental and subject to change.

8.7.1 SUNMatrix_cuSparse functions

The SUNMATRIX_CUSPARSE module defines GPU-enabled sparse implementations of all matrix operations listed in Section 8.1.1 except for the SUNMatSpace and SUNMatMatvecSetup operations:

1. SUNMatGetID_cuSparse – returns SUNMATRIX_CUSPARSE
2. SUNMatClone_cuSparse
3. SUNMatDestroy_cuSparse
4. SUNMatZero_cuSparse
5. SUNMatCopy_cuSparse
6. SUNMatScaleAdd_cuSparse – performs $A = cA+B$, where A and B must have the same sparsity pattern
7. SUNMatScaleAddI_cuSparse – performs $A = cA + I$, where the diagonal of A must be present
8. SUNMatMatvec_cuSparse

In addition, the SUNMATRIX_CUSPARSE module defines the following implementation specific functions:

SUNMatrix_cuSparse_NewCSR

Call `A = SUNMatrix_cuSparse_NewCSR(M, N, NNZ, cusp)`

Description This constructor function creates and allocates memory for a SUNMATRIX_CUSPARSE SUNMatrix that uses the CSR storage format.

Arguments
- `M` (int) the number of matrix rows
- `N` (int) the number of matrix columns

NNZ (int) the number of matrix nonzeros
cusp (cusparseHandle_t) a valid cusparseHandle_t

Return value a SUNMatrix object if successful else NULL

SUNMatrix_cuSparse_NewBlockCSR

Call `A = SUNMatrix_cuSparse_NewBlockCSR(nblocks, blockrows, blockcols, blocknnz, cusp)`

Description This constructor function creates and allocates memory for a SUNMATRIX_CUSPARSE SUNMatrix that leverages the SUNMAT_CUSPARSE_BCSR storage format to store a block diagonal matrix where each block shares the same sparsity pattern. **The blocks must be square.**

Arguments
nblocks (int) the number of matrix blocks
blockrows (int) the number of rows for a block
blockcols (int) the number of columns for a block
blocknnz (int) the number of nonzeros in a block
cusp a valid cusparseHandle_t

Return value a SUNMatrix object if successful else NULL

Notes The SUNMAT_CUSPARSE_BCSR format currently only supports square matrices.

SUNMatrix_cuSparse_MakeCSR

Call `A = SUNMatrix_cuSparse_MakeCSR(mat_descr, M, N, NNZ, rowptrs, colind, data, cusp)`

Description This constructor function creates and allocates memory for a SUNMATRIX_CUSPARSE SUNMatrix that uses the CSR storage format from the user provided pointers.

Arguments
mat_decsr a valid cusparseMatDescr_t object; must use CUSPARSE_INDEX_BASE_ZERO indexing
M (int) the number of matrix rows
N (int) the number of matrix columns
NNZ (int) the number of matrix nonzeros
rowptrs (int*)a contiguous array of the CSR row pointers
colind (int*) a contiguous array of the CSR column indices
data (realtype*) a contiguous array of the nonzero data
cusp (cusparseHandle_t) a valid cusparseHandle_t

Return value a SUNMatrix object if successful else NULL

SUNMatrix_cuSparse_Rows

Call `M = SUNMatrix_cuSparse_Rows(A)`

Description This function returns the number of rows in the sparse SUNMatrix.

Arguments A (SUNMatrix)

Return value the number of rows in the sparse SUNMatrix

SUNMatrix_cuSparse_Columns

Call `N = SUNMatrix_cuSparse_Columns(A)`

Description This function returns the number of columns in the sparse SUNMatrix.

Arguments A (SUNMatrix)

Return value the number of columns in the sparse SUNMatrix

`SUNMatrix_cuSparse_NNZ`

Call `nnz = SUNMatrix_cuSparse_NNZ(A)`

Description This function returns the number of nonzeros in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of nonzeros in the sparse `SUNMatrix`

`SUNMatrix_cuSparse_SparseType`

Call `type = SUNMatrix_cuSparse_SparseType(A)`

Description This function returns the sparsity format for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the `SUNMAT_CUSPARSE_CSR` or `SUNMAT_CUSPARSE_BCSR` sparsity formats

`SUNMatrix_cuSparse_IndexValues`

Call `colind = SUNMatrix_cuSparse_IndexValues(A)`

Description This function returns a pointer to the index value array for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value for the CSR format this is an array of the column indices for each nonzero entry. For the BCSR format this is an array of the column indices for each nonzero entry in the first block only.

`SUNMatrix_cuSparse_IndexPointers`

Call `rowptrs = SUNMatrix_cuSparse_IndexPointers(A)`

Description This function returns a pointer to the index pointers array for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value for the CSR format this is an array of the locations of the first entry of each row in the `data` and `indexvalues` arrays, for the BCSR format this is an array of the locations of each row in the `data` and `indexvalues` arrays in the first block only.

`SUNMatrix_cuSparse_NumBlocks`

Call `nblocks = SUNMatrix_cuSparse_NumBlocks(A)`

Description This function returns the number of blocks in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of matrix blocks

`SUNMatrix_cuSparse_BlockRows`

Call `blockrows = SUNMatrix_cuSparse_BlockRows(A)`

Description This function returns the number of rows of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of rows of a block

`SUNMatrix_cuSparse_BlockColumns`

Call `blockrows = SUNMatrix_cuSparse_BlockColumns(A)`

Description This function returns the number of columns of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of columns of a block

`SUNMatrix_cuSparse_BlockNNZ`

Call `blockdim = SUNMatrix_cuSparse_BlockNNZ(A)`

Description This function returns the nonzeros of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of nonzeros of a block

`SUNMatrix_cuSparse_BlockData`

Call `nzdata = SUNMatrix_cuSparse_BlockData(A, blockidx)`

Description This function returns a pointer to the start of the nonzero values in the data array for given block index. The first block in the `SUNMatrix` is index 0, the second block is index 1, and so on.

Arguments `A` (`SUNMatrix`)
`blockidx` (`int`) the index of the desired block

Return value a pointer to the start of the nonzero values in the data array for given block index

`SUNMatrix_cuSparse_CopyToDevice`

Call `retval = SUNMatrix_cuSparse_CopyToDevice(A, h_data, h_idxptrs, h_idxvals)`

Description This functions copies the matrix information to the GPU device from the provided host arrays. A user may provide `NULL` for any of `h_data`, `h_idxptrs`, or `h_idxvals` to avoid copying that information.

Arguments `A` (`SUNMatrix`)
`h_data` (`realtype*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_NNZ(A) * sizeof(realtype)` bytes; the nonzero values will be copied from this array onto the device
`h_idxptrs` (`int*`) a pointer to an allocated array of at least `(SUNMatrix_cuSparse_BlockDim(A)+1) * sizeof(int)` bytes; the index pointers will be copied from this array onto the device
`h_idxvals` (`int*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_BlockNNZ(A) * sizeof(int)` bytes; the index values will be copied from this array onto the device

Return value `SUNMAT_SUCCESS` if the copy operation(s) were successful, or a nonzero error code otherwise.

`SUNMatrix_cuSparse_CopyFromDevice`

Call `retval = SUNMatrix_cuSparse_CopyFromDevice(A, h_data, h_idxptrs, h_idxvals)`

Description This functions copies the matrix information from the GPU device to the provided host arrays. A user may provide `NULL` for any of `h_data`, `h_idxptrs`, or `h_idxvals` to avoid copying that information.

Arguments `A` (`SUNMatrix`)

`h_data` (`realtype*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_NNZ(A) * sizeof(realtype)` bytes; the nonzero values will be copied into this array from the device

`h_idxptrs` (`int*`) a pointer to an allocated array of at least `(SUNMatrix_cuSparse_BlockDim(A)+1) * sizeof(int)` bytes; the index pointers will be copied into this array from the device

`h_idxvals` (`int*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_BlockNNZ(A) * sizeof(int)` bytes; the index values will be copied into this array from the device

Return value `SUNMAT_SUCCESS` if the copy operation(s) were successful, or a nonzero error code otherwise.

`SUNMatrix_cuSparse_SetKernelExecPolicy`

Call `retval = SUNMatrix_cuSparse_SetKernelExecPolicy(A, exec_policy);`

Description This function sets the execution policies which control the kernel parameters utilized when launching the CUDA kernels. By default the matrix is setup to use a policy which tries to leverage the structure of the matrix. See section 7.9.2 for more information about the `SUNCudaExecPolicy` class.

Arguments `A` (`SUNMatrix`)
`exec_policy` (`SUNCudaExecPolicy*`)

Return value `SUNMAT_SUCCESS` if the operation(s) were successful, or a nonzero error code otherwise.

Notes All matrices and vector 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.

`SUNMatrix_cuSparse_SetFixedPattern`

Call `retval = SUNMatrix_cuSparse_SetFixedPattern(A, yesno)`

Description This function changes the behavior of the the `SUNMatZero` operation on the `SUNMatrix` object `A`. By default the matrix sparsity pattern is not considered to be fixed, thus, the `SUNMatZero` operation zeros out all `data` array as well as the `indexvalues` and `indexpointers` arrays. Providing a value of `1` or `SUNTRUE` for the `yesno` argument changes the behavior of `SUNMatZero` on `A` so that only the data is zeroed out, but not the `indexvalues` or `indexpointers` arrays. Providing a value of `0` or `SUNFALSE` for the `yesno` argument is equivalent to the default behavior.

Arguments `A` (`SUNMatrix`)
`yesno` (`booleantype`)

Return value `SUNMAT_SUCCESS` if the operation(s) were successful, or a nonzero error code otherwise.

8.7.2 SUNMatrix_cuSparse Usage Notes

The `SUNMATRIX_CUSPARSE` module only supports 32-bit indexing, thus SUNDIALS must be built for 32-bit indexing to use this module.

The `SUNMATRIX_CUSPARSE` module can be used with CUDA streams by calling the cuSPARSE function `cusparseSetStream` on the the `cusparseHandle_t` that is provided to the `SUNMATRIX_CUSPARSE` constructor.

When using the `SUNMATRIX_CUSPARSE` module with a SUNDIALS package (e.g. CVODE), the stream given to cuSPARSE should be the same stream used for the NVECTOR object that is provided to the package, and the NVECTOR object given to the `SUNMatvec` operation. If different streams are utilized, synchronization issues may occur.

8.8 The SUNMATRIX_MAGMADENSE implementation

The SUNMATRIX_MAGMADENSE implementation of the SUNDIALS SUNMatrix API interfaces to the MAGMA () linear algebra library, and can target NVIDIA's CUDA programming model or AMD's HIP programming model [45]. All data stored by this matrix implementation resides on the GPU at all times. The implementation currently supports a standard LAPACK column-major storage format as well as a low-storage format for block-diagonal matrices

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix}.$$

This matrix implementation is best paired with the SUNLINEARSOLVER_MAGMADENSE SUNLinearSolver.

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

The SUNMATRIX_MAGMADENSE module is experimental and subject to change.

8.8.1 SUNMATRIX_MAGMADENSE functions

The SUNMATRIX_MAGMADENSE module defines GPU-enabled implementations of all matrix operations listed in Section 8.1.1.

1. SUNMatGetID_MagmaDense – returns SUNMATRIX_MAGMADENSE
2. SUNMatClone_MagmaDense
3. SUNMatDestroy_MagmaDense
4. SUNMatZero_MagmaDense
5. SUNMatCopy_MagmaDense
6. SUNMatScaleAdd_MagmaDense
7. SUNMatScaleAddI_MagmaDense
8. SUNMatMatvecSetup_MagmaDense
9. SUNMatMatvec_MagmaDense
10. SUNMatSpace_MagmaDense

In addition, the SUNMATRIX_MAGMADENSE module defines the following implementation specific functions:

SUNMatrix_MagmaDense

Call `A = SUNMatrix_MagmaDense(M, N, memtype, memhelper, queue)`

Description This constructor function creates and allocates memory for an $M \times N$ SUNMATRIX_MAGMADENSE SUNMatrix.

Arguments

`M`	(sunindextype) the number of matrix rows
`N`	(sunindextype) the number of matrix columns
`memtype`	(SUNMemoryType) the type of memory to use for the matrix data; can be SUNMEMTYPE_UVM or SUNMEMTYPE_DEVICE.
`memhelper`	(SUNMemoryHelper) the memory helper used for allocating data
`queue`	a cudaStream_t when using CUDA or a hipStream_t when using HIP

Return value A SUNMatrix object if successful else NULL.

`SUNMatrix_MagmaDenseBlock`

Call `A = SUNMatrix_MagmaDenseBlock(nblocks, M_block, N_block, memtype, memhelper, queue)`

Description This constructor function creates and allocates memory for a `SUNMATRIX_MAGMADENSE` `SUNMatrix` that is block diagonal with `nblocks` blocks of size $M \times N$.

Arguments
- `nblocks` (`sunindextype`) the number of matrix blocks
- `M_block` (`sunindextype`) the number of matrix rows in each block
- `N_block` (`sunindextype`) the number of matrix columns in each block
- `memtype` (`SUNMemoryType`) the type of memory to use for the matrix data; can be `SUNMEMTYPE_UVM` or `SUNMEMTYPE_DEVICE`.
- `memhelper` (`SUNMemoryHelper`) the memory helper used for allocating data
- `queue` a `cudaStream_t` when using CUDA or a `hipStream_t` when using HIP

Return value A `SUNMatrix` object if successful else `NULL`.

Notes The block diagonal format currently supports square matrices only.

`SUNMatrix_MagmaDense_Rows`

Call `M = SUNMatrix_MagmaDense_Rows(A)`

Description This function returns the rows dimension for the $M \times N$ `SUNMatrix`. For block diagonal matrices, this is computed as $M_{\text{block}} \times$ nblocks.

Arguments `A` (`SUNMatrix`)

Return value The number of rows in the `SUNMatrix`.

`SUNMatrix_MagmaDense_Columns`

Call `N = SUNMatrix_MagmaDense_Columns(A)`

Description This function returns the columns dimension for the $M \times N$ `SUNMatrix`. For block diagonal matrices, this is computed as $N_{\text{block}} \times$ nblocks.

Arguments `A` (`SUNMatrix`)

Return value The number of columns in the `SUNMatrix`.

`SUNMatrix_MagmaDense_BlockRows`

Call `M = SUNMatrix_MagmaDense_BlockRows(A)`

Description This function returns the number of rows in a block of the `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value The number of rows in a block of the `SUNMatrix`.

`SUNMatrix_MagmaDense_BlockColumns`

Call `N = SUNMatrix_MagmaDense_BlockColumns(A)`

Description This function returns the number of columns in a block of the `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value The number of columns in a block of the `SUNMatrix`.

`SUNMatrix_MagmaDense_LData`

Call `ldata = SUNMatrix_MagmaDense_LData(A)`

Description This function returns the length of the data array for the `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value The length of the data array for the `SUNMatrix`.

`SUNMatrix_MagmaDense_NumBlocks`

Call `nblocks = SUNMatrix_MagmaDense_NumBlocks(A)`

Description This function returns the number of blocks in the `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value The number of matrix blocks.

`SUNMatrix_MagmaDense_Data`

Call `data = SUNMatrix_MagmaDense_Data(A)`

Description This function returns the `SUNMatrix` data array.

Arguments `A` (`SUNMatrix`)

Return value An array of pointers to the data arrays for each block in the `SUNMatrix`.

`SUNMatrix_MagmaDense_BlockData`

Call `data = SUNMatrix_MagmaDense_BlockData(A)`

Description This function returns an array of pointers that point to the start of the data array for each block.

Arguments `A` (`SUNMatrix`)

Return value An array of pointers to the data arrays for each block in the `SUNMatrix`.

`SUNMatrix_MagmaDense_Block`

Call `data = SUNMatrix_MagmaDense_Block(A, k)`

Description This function returns a pointer to the data for block k.

Arguments `A` (`SUNMatrix`)

Return value A pointer to the start of the data array for block k in the `SUNMatrix`.

Notes No bounds-checking is performed, k should be stricly less than nblocks.

`SUNMatrix_MagmaDense_Column`

Call `data = SUNMatrix_MagmaDense_Column(A, j)`

Description This function returns a pointer to the data for column j of the matrix.

Arguments `A` (`SUNMatrix`)

Return value A pointer to the start of the data array for column j of the `SUNMatrix`.

Notes No bounds-checking is performed, j should be stricly less than nblocks $* N_{\text{block}}$.

`SUNMatrix_MagmaDense_BlockColumn`

Call `data = SUNMatrix_MagmaDense_Column(A, k, j)`

Description This function returns a pointer to the data for column j of block k.

Arguments `A` (`SUNMatrix`)

Return value A pointer to the start of the data array for column j of block k in the `SUNMatrix`.

Notes No bounds-checking is performed.

`SUNMatrix_MagmaDense_CopyToDevice`

Call `retval = SUNMatrix_MagmaDense_CopyToDevice(A, h_data)`

Description This functions copies the matrix data to the GPU device from the provided host array.

Arguments `A` (`SUNMatrix`)
`h_data` (`realtype*`)

Return value `SUNMAT_SUCCESS` if the copy operation was successful, or a nonzero error code otherwise

`SUNMatrix_MagmaDense_CopyFromDevice`

Call `retval = SUNMatrix_MagmaDense_CopyFromDevice(A, h_data)`

Description This functions copies the matrix data from the GPU device to the provided host array.

Arguments `A` (`SUNMatrix`)
`h_data` (`realtype*`)

Return value `SUNMAT_SUCCESS` if the copy operation was successful, or a nonzero error code otherwise

8.8.2 SUNMATRIX_MAGMADENSE Usage Notes

When using the `SUNMATRIX_MAGMADENSE` module with a SUNDIALS package (e.g. CVODE), the stream given to matrix should be the same stream used for the NVECTOR object that is provided to the package, and the NVECTOR object given to the `SUNMatvec` operation. If different streams are utilized, synchronization issues may occur.

Chapter 9

Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS packages operate using generic linear solver modules defined through the SUNLINSOL API. This allows SUNDIALS packages to utilize any valid SUNLINSOL implementation that provides a set of required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group consists of "set" routines to supply the linear solver object with functions provided by the SUNDIALS package, or for modification of solver parameters. The last group consists of "get" routines for retrieving artifacts (statistics, residual vectors, etc.) from the linear solver. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

The implementations provided with SUNDIALS work in coordination with the SUNDIALS generic NVECTOR and SUNMATRIX modules to provide a set of compatible data structures and solvers for the solution of linear systems using direct or iterative (matrix-based or matrix-free) methods. Moreover, advanced users can provide a customized `SUNLinearSolver` implementation to any SUNDIALS package, particularly in cases where they provide their own NVECTOR and/or SUNMATRIX modules.

Historically, the SUNDIALS packages have been designed to specifically leverage the use of either *direct linear solvers* or matrix-free, *scaled, preconditioned, iterative linear solvers*. However, matrix-based iterative linear solvers are also supported.

The iterative linear solvers packaged with SUNDIALS leverage scaling and preconditioning, as applicable, to balance error between solution components and to accelerate convergence of the linear solver. To this end, instead of solving the linear system $Ax = b$ directly, these apply the underlying iterative algorithm to the transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.1}$$

where

$$\begin{aligned} \tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\ \tilde{b} &= S_1 P_1^{-1} b, \\ \tilde{x} &= S_2 P_2 x, \end{aligned} \tag{9.2}$$

and where

- P_1 is the left preconditioner,
- P_2 is the right preconditioner,
- S_1 is a diagonal matrix of scale factors for $P_1^{-1} b$,
- S_2 is a diagonal matrix of scale factors for $P_2 x$.

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

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

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 9.1.1 – 9.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 9.1.4. A table of linear solver return codes is given in section 9.1.5. The `SUNLinearSolver` type and the generic SUNLINSOL module are defined in section 9.1.6. The section 9.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 9.3 lists the requirements for supplying a custom SUNLINSOL module and discusses some intended use cases. Users wishing to supply their own SUNLINSOL module are encouraged to use the SUNLINSOL implementations provided with SUNDIALS as a template for supplying custom linear solver modules. The SUNLINSOL functions required by this SUNDIALS package as well as other package specific details are given in section 9.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

9.1 The SUNLinearSolver API

The SUNLINSOL API defines several linear solver operations that enable SUNDIALS packages to utilize any SUNLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group of functions consists of set routines to supply the linear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving linear solver statistics. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

9.1.1 `SUNLinearSolver` core functions

The core linear solver functions consist of two required functions to get the linear solver type (`SUNLinSolGetType`) and solve the linear system $Ax = b$ (`SUNLinSolSolve`). The remaining functions are for getting the solver ID (`SUNLinSolGetID`), initializing the linear solver object once all solver-specific options have been set (`SUNLinSolInitialize`), setting up the linear solver object to utilize an updated matrix A (`SUNLinSolSetup`), and for destroying the linear solver object (`SUNLinSolFree`) are optional.

SUNLinSolGetType

Call `type = SUNLinSolGetType(LS);`

Description The *required* function `SUNLinSolGetType` returns the type identifier for the linear solver `LS`. It is used to determine the solver type (direct, iterative, or matrix-iterative) from the abstract `SUNLinearSolver` interface.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

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

- `SUNLINEARSOLVER_DIRECT` – `0`, the SUNLINSOL module requires a matrix, and computes an 'exact' solution to the linear system defined by that matrix.
- `SUNLINEARSOLVER_ITERATIVE` – `1`, the SUNLINSOL module does not require a matrix (though one may be provided), and computes an inexact solution to the linear system using a matrix-free iterative algorithm. That is it solves the linear system defined by the package-supplied `ATimes` routine (see `SUNLinSolSetATimes` below), even if that linear system differs from the one encoded in the matrix object (if one is provided). As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.
- `SUNLINEARSOLVER_MATRIX_ITERATIVE` – `2`, the SUNLINSOL module requires a matrix, and computes an inexact solution to the linear system defined by that matrix using an iterative algorithm. That is it solves the linear system defined by the matrix object even if that linear system differs from that encoded by the package-supplied `ATimes` routine. As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.

Notes See section 9.3.1 for more information on intended use cases corresponding to the linear solver type.

F2003 Name `FSUNLinSolGetType`

SUNLinSolGetID

Call `id = SUNLinSolGetID(LS);`

Description The *optional* function `SUNLinSolGetID` returns the identifier for the linear solver `LS`.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value The return value `id` (of type `int`) will be a non-negative value defined by the enumeration `SUNLinearSolver_ID`.

Notes It is recommended that a user-supplied `SUNLinearSolver` return the `SUNLINEARSOLVER_CUSTOM` identifier.

F2003 Name `FSUNLinSolGetID`

SUNLinSolInitialize

Call `retval = SUNLinSolInitialize(LS);`

Description The *optional* function `SUNLinSolInitialize` performs linear solver initialization (assuming that all solver-specific options have been set).

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value This should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.1.

F2003 Name `FSUNLinSolInitialize`

`SUNLinSolSetup`

Call `retval = SUNLinSolSetup(LS, A);`

Description The *optional* function `SUNLinSolSetup` performs any linear solver setup needed, based on an updated system SUNMATRIX `A`. This may be called frequently (e.g., with a full Newton method) or infrequently (for a modified Newton method), based on the type of integrator and/or nonlinear solver requesting the solves.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`A` (`SUNMatrix`) a SUNMATRIX object.

Return value This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 9.1.

F2003 Name `FSUNLinSolSetup`

`SUNLinSolSolve`

Call `retval = SUNLinSolSolve(LS, A, x, b, tol);`

Description The *required* function `SUNLinSolSolve` solves a linear system $Ax = b$.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`A` (`SUNMatrix`) a SUNMATRIX object.

`x` (`N_Vector`) a NVECTOR object containing the initial guess for the solution of the linear system, and the solution to the linear system upon return.

`b` (`N_Vector`) a NVECTOR object containing the linear system right-hand side.

`tol` (`realtype`) the desired linear solver tolerance.

Return value This should return zero for a successful call, a positive value for a recoverable failure and a negative value for an unrecoverable failure, ideally returning one of the generic error codes listed in Table 9.1.

Notes **Direct solvers:** can ignore the `tol` argument.

Matrix-free solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE`) can ignore the SUNMATRIX input `A`, and should instead rely on the matrix-vector product function supplied through the routine `SUNLinSolSetATimes`.

Iterative solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`) should attempt to solve to the specified tolerance `tol` in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.

F2003 Name `FSUNLinSolSolve`

`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.

F2003 Name `FSUNLinSolFree`

9.1.2 SUNLinearSolver set functions

The following set functions are used to supply linear solver modules with functions defined by the SUNDIALS packages and to modify solver parameters. Only the routine for setting the matrix-vector product routine is required, and that is only for matrix-free linear solver modules. Otherwise, all other set functions are optional. SUNLINSOL implementations that do not provide the functionality for any optional routine should leave the corresponding function pointer `NULL` instead of supplying a dummy routine.

`SUNLinSolSetATimes`

Call `retval = SUNLinSolSetATimes(LS, A_data, ATimes);`

Description The function `SUNLinSolSetATimes` is *required for matrix-free linear solvers*; otherwise it is optional.

This routine provides an `ATimesFn` function pointer, as well as a `void*` pointer to a data structure used by this routine, to a linear solver object. SUNDIALS packages will call this function to set the matrix-vector product function to either a solver-provided difference-quotient via vector operations or a user-supplied solver-specific routine.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`A_data` (`void*`) data structure passed to `ATimes`.

`ATimes` (`ATimesFn`) function pointer implementing the matrix-vector product routine.

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.1.

F2003 Name `FSUNLinSolSetATimes`

`SUNLinSolSetPreconditioner`

Call `retval = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);`

Description The *optional* function `SUNLinSolSetPreconditioner` provides `PSetupFn` and `PSolveFn` function pointers that implement the preconditioner solves P_1^{-1} and P_2^{-1} from equations (9.1)-(9.2). This routine will be called by a SUNDIALS package, which will provide translation between the generic `Pset` and `Psol` calls and the package- or user-supplied routines.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`Pdata` (`void*`) data structure passed to both `Pset` and `Psol`.

`Pset` (`PSetupFn`) function pointer implementing the preconditioner setup.

`Psol` (`PSolveFn`) function pointer implementing the preconditioner solve.

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.1.

F2003 Name `FSUNLinSolSetPreconditioner`

`SUNLinSolSetScalingVectors`

Call `retval = SUNLinSolSetScalingVectors(LS, s1, s2);`

Description The *optional* function `SUNLinSolSetScalingVectors` provides left/right scaling vectors for the linear system solve. Here, `s1` and `s2` are NVECTOR of positive scale factors containing the diagonal of the matrices S_1 and S_2 from equations (9.1)-(9.2), respectively. Neither of these vectors need to be tested for positivity, and a `NULL` argument for either indicates that the corresponding scaling matrix is the identity.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

`s1` (`N_Vector`) diagonal of the matrix S_1

`s2` (`N_Vector`) diagonal of the matrix S_2

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.1.

F2003 Name `FSUNLinSolSetScalingVectors`

9.1.3 SUNLinearSolver get functions

The following get functions allow SUNDIALS packages to retrieve results from a linear solve. All routines are optional.

`SUNLinSolNumIters`

Call `its = SUNLinSolNumIters(LS);`

Description The *optional* function `SUNLinSolNumIters` should return the number of linear iterations performed in the last 'solve' call.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.

Return value `int` containing the number of iterations

F2003 Name `FSUNLinSolNumIters`

`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

F2003 Name `FSUNLinSolResNorm`

`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.

F2003 Name `FSUNLinSolResid`

`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 `sunindextype` containing the most recent error flag

F2003 Name `FSUNLinSolLastFlag`

`SUNLinSolSpace`

Call `retval = SUNLinSolSpace(LS, &lrw, &liw);`

Description The *optional* function `SUNLinSolSpace` should return the storage requirements for the linear solver `LS`.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`lrw` (`long int*`) the number of realtype words stored by the linear solver.
`liw` (`long int*`) the number of integer words stored by the linear solver.

Return value This should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 9.1.

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

F2003 Name `FSUNLinSolSpace`

9.1.4 Functions provided by SUNDIALS packages

To interface with the SUNLINSOL modules, the SUNDIALS packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic interfaces to the linear systems of equations that result in their solution. The types for functions provided to a SUNLINSOL module are defined in the header file `sundials/sundials_iterative.h`, and are described below.

`ATimesFn`

Definition `typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);`

Purpose These functions compute the action of a matrix on a vector, performing the operation $z = Av$. Memory for `z` should already be allocted prior to calling this function. The vector `v` should be left unchanged.

Arguments `A_data` is a pointer to client data, the same as that supplied to `SUNLinSolSetATimes`.
`v` is the input vector to multiply.
`z` is the output vector computed.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

`PSetupFn`

Definition `typedef int (*PSetupFn)(void *P_data)`

Purpose These functions set up any requisite problem data in preparation for calls to the corresponding `PSolveFn`.

Arguments `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

PSolveFn

Definition
```
typedef int (*PSolveFn)(void *P_data, N_Vector r, N_Vector z,
                        realtype tol, int lr)
```

Purpose These functions solve the preconditioner equation $Pz = r$ for the vector z. Memory for `z` should already be allocted prior to calling this function. The parameter `P_data` is a pointer to any information about P which the function needs in order to do its job (set up by the corresponding `PSetupFn`). The parameter `lr` is input, and indicates whether P is to be taken as the left preconditioner or the right preconditioner: `lr` $= 1$ for left and `lr` $= 2$ for right. If preconditioning is on one side only, `lr` can be ignored. If the preconditioner is iterative, then it should strive to solve the preconditioner equation so that

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

where the weight vector for the WRMS norm may be accessed from the main package memory structure. The vector `r` should not be modified by the `PSolveFn`.

Arguments
- `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.
- `r` is the right-hand side vector for the preconditioner system.
- `z` is the solution vector for the preconditioner system.
- `tol` is the desired tolerance for an iterative preconditioner.
- `lr` is flag indicating whether the routine should perform left (1) or right (2) preconditioning.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful. On a failure, a negative return value indicates an unrecoverable condition, while a positive value indicates a recoverable one, in which the calling routine may reattempt the solution after updating preconditioner data.

9.1.5 `SUNLinearSolver` return codes

The functions provided to SUNLINSOL modules by each SUNDIALS package, and functions within the SUNDIALS-provided SUNLINSOL implementations utilize a common set of return codes, shown in Table 9.1. These adhere to a common pattern: 0 indicates success, a postitive value corresponds to a recoverable failure, and a negative value indicates a non-recoverable failure. Aside from this pattern, the actual values of each error code are primarily to provide additional information to the user in case of a linear solver failure.

Table 9.1: Description of the `SUNLinearSolver` error codes

Name	Value	Description
SUNLS_SUCCESS	0	successful call or converged solve
SUNLS_MEM_NULL	-801	the memory argument to the function is NULL
SUNLS_ILL_INPUT	-802	an illegal input has been provided to the function
SUNLS_MEM_FAIL	-803	failed memory access or allocation
SUNLS_ATIMES_NULL	-804	the Atimes function is NULL

continued on next page

Name	Value	Description
SUNLS_ATIMES_FAIL_UNREC	-805	an unrecoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_UNREC	-806	an unrecoverable failure occurred in the Pset routine
SUNLS_PSOLVE_NULL	-807	the preconditioner solve function is NULL
SUNLS_PSOLVE_FAIL_UNREC	-808	an unrecoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_UNREC	-809	an unrecoverable failure occurred in an external linear solver package
SUNLS_GS_FAIL	-810	a failure occurred during Gram-Schmidt orthogonalization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_QRSOL_FAIL	-811	a singular R matrix was encountered in a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_VECTOROP_ERR	-812	a vector operation error occurred
SUNLS_RES_REDUCED	801	an iterative solver reduced the residual, but did not converge to the desired tolerance
SUNLS_CONV_FAIL	802	an iterative solver did not converge (and the residual was not reduced)
SUNLS_ATIMES_FAIL_REC	803	a recoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_REC	804	a recoverable failure occurred in the Pset routine
SUNLS_PSOLVE_FAIL_REC	805	a recoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_REC	806	a recoverable failure occurred in an external linear solver package
SUNLS_QRFACT_FAIL	807	a singular matrix was encountered during a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_LUFACT_FAIL	808	a singular matrix was encountered during a LU factorization (SUNLINSOL_DENSE/SUNLINSOL_BAND)

9.1.6 The generic SUNLinearSolver module

SUNDIALS packages interact with specific SUNLINSOL implementations through the generic SUNLINSOL module on which all other SUNLINSOL iplementations are built. The SUNLinearSolver type is a pointer to a structure containing an implementation-dependent *content* field, and an *ops* field. The type SUNLinearSolver is defined as

```
typedef struct _generic_SUNLinearSolver *SUNLinearSolver;

struct _generic_SUNLinearSolver {
  void *content;
  struct _generic_SUNLinearSolver_Ops *ops;
};
```

where the _generic_SUNLinearSolver_Ops structure is a list of pointers to the various actual linear solver operations provided by a specific implementation. The _generic_SUNLinearSolver_Ops structure is defined as

```
struct _generic_SUNLinearSolver_Ops {
  SUNLinearSolver_Type (*gettype)(SUNLinearSolver);
  SUNLinearSolver_ID   (*getid)(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);
  sunindxetype         (*lastflag)(SUNLinearSolver);
  int                  (*space)(SUNLinearSolver, long int*, long int*);
  N_Vector             (*resid)(SUNLinearSolver);
  int                  (*free)(SUNLinearSolver);
};
```

The generic SUNLINSOL module defines and implements the linear solver operations defined in Sections 9.1.1-9.1.3. These routines are in fact only wrappers to the linear solver operations defined by a particular SUNLINSOL implementation, which are accessed through the *ops* field of the `SUNLinearSolver` structure. To illustrate this point we show below the implementation of a typical linear solver operation from the generic SUNLINSOL module, namely `SUNLinSolInitialize`, which initializes a SUNLINSOL object for use after it has been created and configured, and returns a flag denoting a successful/failed operation:

```
int SUNLinSolInitialize(SUNLinearSolver S)
{
  return ((int) S->ops->initialize(S));
}
```

The Fortran 2003 interface provides a `bind(C)` derived-type for the `_generic_SUNLinearSolver` and the `_generic_SUNLinearSolver_Ops` structures. Their definition is given below.

```
 type, bind(C), public :: SUNLinearSolver
  type(C_PTR), public :: content
  type(C_PTR), public :: ops
 end type SUNLinearSolver

 type, bind(C), public :: SUNLinearSolver_Ops
  type(C_FUNPTR), public :: gettype
  type(C_FUNPTR), public :: setatimes
  type(C_FUNPTR), public :: setpreconditioner
  type(C_FUNPTR), public :: setscalingvectors
  type(C_FUNPTR), public :: initialize
  type(C_FUNPTR), public :: setup
  type(C_FUNPTR), public :: solve
  type(C_FUNPTR), public :: numiters
  type(C_FUNPTR), public :: resnorm
  type(C_FUNPTR), public :: lastflag
  type(C_FUNPTR), public :: space
  type(C_FUNPTR), public :: resid
  type(C_FUNPTR), public :: free
 end type SUNLinearSolver_Ops
```

9.2 Compatibility of `SUNLinearSolver` modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 9.2 we show the matrix-based linear solvers available as SUNLINSOL modules,

and the compatible matrix implementations. Recall that Table 4.1 shows the compatibility between all SUNLINSOL modules and vector implementations.

Table 9.2: SUNDIALS matrix-based linear solvers and matrix implementations that can be used for each.

Linear Solver Interface	Dense Matrix	Banded Matrix	Sparse Matrix	SLUNRloc Matrix	User Supplied
Dense	✓				✓
Band		✓			✓
LapackDense	✓				✓
LapackBand		✓			✓
KLU			✓		✓
SuperLU_DIST				✓	✓
SUPERLUMT			✓		✓
User supplied	✓	✓	✓	✓	✓

9.3 Implementing a custom SUNLinearSolver module

A particular implementation of the SUNLINSOL module must:

- Specify the *content* field of the `SUNLinearSolver` object.
- Define and implement a minimal subset of the linear solver operations. See the section 9.4 to determine which SUNLINSOL operations are required for this SUNDIALS package.

  Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNLINSOL module (each with different `SUNLinearSolver` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free a `SUNLinearSolver` with the new *content* field and with *ops* pointing to the new linear solver operations.

We note that the function pointers for all unsupported optional routines should be set to `NULL` in the *ops* structure. This allows the SUNDIALS package that is using the SUNLINSOL object to know that the associated functionality is not supported.

To aid in the creation of custom SUNLINSOL modules the generic SUNLINSOL module provides the utility functions `SUNLinSolNewEmpty` and `SUNLinSolFreeEmpty`. When used in custom SUNLINSOL constructors the function `SUNLinSolNewEmpty` will ease the introduction of any new optional linear solver operations to the SUNLINSOL API by ensuring only required operations need to be set.

`SUNLinSolNewEmpty`

Call `LS = SUNLinSolNewEmpty();`

Description The function `SUNLinSolNewEmpty` allocates a new generic SUNLINSOL object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

Arguments None

Return value This function returns a `SUNLinearSolver` object. If an error occurs when allocating the object, then this routine will return `NULL`.

F2003 Name `FSUNLinSolNewEmpty`

`SUNLinSolFreeEmpty`

Call `SUNLinSolFreeEmpty(LS);`

Description This routine frees the generic `SUNLinSolFreeEmpty` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `LS` (`SUNLinearSolver`)

Return value None

F2003 Name `FSUNLinSolFreeEmpty`

Additionally, a SUNLINSOL implementation *may* do the following:

- Define and implement additional user-callable "set" routines acting on the `SUNLinearSolver`, e.g., for setting various configuration options to tune the linear solver to a particular problem.
- Provide additional user-callable "get" routines acting on the `SUNLinearSolver` object, e.g., for returning various solve statistics.

9.3.1 Intended use cases

The SUNLINSOL (and SUNMATRIX) APIs are designed to require a minimal set of routines to ease interfacing with custom or third-party linear solver libraries. External solvers provide similar routines with the necessary functionality and thus will require minimal effort to wrap within custom SUNMATRIX and SUNLINSOL implementations. Sections 8.2 and 9.4 include a list of the required set of routines that compatible SUNMATRIX and SUNLINSOL implementations must provide. As SUNDIALS packages utilize generic SUNLINSOL modules allowing for user-supplied `SUNLinearSolver` implementations, there exists a wide range of possible linear solver combinations. Some intended use cases for both the SUNDIALS-provided and user-supplied SUNLINSOL modules are discussd in the following sections.

Direct linear solvers

Direct linear solver modules require a matrix and compute an 'exact' solution to the linear system *defined by the matrix*. Multiple matrix formats and associated direct linear solvers are supplied with SUNDIALS through different SUNMATRIX and SUNLINSOL implementations. SUNDIALS packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations. As a result, each package's linear solver interface recomputes Jacobian information as infrequently as possible.

Alternative matrix storage formats and compatible linear solvers that are not currently provided by, or interfaced with, SUNDIALS can leverage this infrastructure with minimal effort. To do so, a user must implement custom SUNMATRIX and SUNLINSOL wrappers for the desired matrix format and/or linear solver following the APIs described in Chapters 8 and 9. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_DIRECT` *type.*

Matrix-free iterative linear solvers

Matrix-free iterative linear solver modules do not require a matrix and compute an inexact solution to the linear system *defined by the package-supplied* `ATimes` *routine*. SUNDIALS supplies multiple scaled, preconditioned iterative linear solver (spils) SUNLINSOL modules that support scaling to allow users to handle non-dimensionalization (as best as possible) within each SUNDIALS package and retain variables and define equations as desired in their applications. For linear solvers that do not support left/right scaling, the tolerance supplied to the linear solver is adjusted to compensate (see section 9.4.2 for more details); however, this use case may be non-optimal and cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single problem.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, SUNDIALS a user must implement a custom SUNLINSOL wrapper for the linear solver following the API

described in Chapter 9. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_ITERATIVE` *type.*

Matrix-based iterative linear solvers (reusing A)

Matrix-based iterative linear solver modules require a matrix and compute an inexact solution to the linear system *defined by the matrix*. This matrix will be updated infrequently and resued across multiple solves to amortize cost of matrix construction. As in the direct linear solver case, only wrappers for the matrix and linear solver in SUNMATRIX and SUNLINSOL implementations need to be created to utilize a new linear solver. *This user-supplied* SUNLINSOL *module must then self-identify as having* `SUNLINEARSOLVER_MATRIX_ITERATIVE` *type.*

At present, SUNDIALS has one example problem that uses this approach for wrapping a structured-grid matrix, linear solver, and preconditioner from the *hypre* library that may be used as a template for other customized implementations (see `examples/arkode/CXX_parhyp/ark_heat2D_hypre.cpp`).

Matrix-based iterative linear solvers (current A)

For users who wish to utilize a matrix-based iterative linear solver module where the matrix is *purely for preconditioning* and the linear system is *defined by the package-supplied* `ATimes` *routine*, we envision two current possibilities.

The preferred approach is for users to employ one of the SUNDIALS spils SUNLINSOL implementations (SUNLINSOL_SPGMR, SUNLINSOL_SPFGMR, SUNLINSOL_SPBCGS, SUNLINSOL_SPTFQMR, or SUNLINSOL_PCG) as the outer solver. The creation and storage of the preconditioner matrix, and interfacing with the corresponding linear solver, can be handled through a package's preconditioner 'setup' and 'solve' functionality (see §4.5.8.2) without creating SUNMATRIX and SUNLINSOL implementations. This usage mode is recommended primarily because the SUNDIALS-provided spils modules support the scaling as described above.

A second approach supported by the linear solver APIs is as follows. If the SUNLINSOL implementation is matrix-based, *self-identifies as having* `SUNLINEARSOLVER_ITERATIVE` *type*, and *also provides a non-*`NULL` `SUNLinSolSetATimes` *routine*, then each SUNDIALS package will call that routine to attach its package-specific matrix-vector product routine to the SUNLINSOL object. The SUNDIALS package will then call the SUNLINSOL-provided `SUNLinSolSetup` routine (infrequently) to update matrix information, but will provide current matrix-vector products to the SUNLINSOL implementation through the package-supplied `ATimesFn` routine.

9.4 IDA SUNLinearSolver interface

Table 9.3 below lists the SUNLINSOL module linear solver functions used within the IDALS interface. As with the SUNMATRIX module, we emphasize that the IDA user does not need to know detailed usage of linear solver functions by the IDA code modules in order to use IDA. The information is presented as an implementation detail for the interested reader.

The linear solver functions listed below are marked with ✓to indicate that they are required, or with † to indicate that they are only called if they are non-`NULL` in the SUNLINSOL implementation that is being used. Note:

1. Although IDALS does not call `SUNLinSolLastFlag` directly, this routine is available for users to query linear solver issues directly.

2. Although IDALS does not call `SUNLinSolFree` directly, this routine should be available for users to call when cleaning up from a simulation.

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.

Table 9.3: List of linear solver function usage in the IDALS interface

	DIRECT	ITERATIVE	MATRIX_ITERATIVE
SUNLinSolGetType	✓	✓	✓
SUNLinSolSetATimes	†	✓	†
SUNLinSolSetPreconditioner	†	†	†
SUNLinSolSetScalingVectors	†	†	†
SUNLinSolInitialize	✓	✓	✓
SUNLinSolSetup	✓	✓	✓
SUNLinSolSolve	✓	✓	✓
SUNLinSolNumIters		✓	✓
SUNLinSolResid		✓	✓
[1]SUNLinSolLastFlag			
[2]SUNLinSolFree			
SUNLinSolSpace	†	†	†

9.4.1 Lagged matrix information

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_DIRECT` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`, then the SUNLINSOL object solves a linear system *defined* by a SUNMATRIX object. IDALS will update the matrix information infrequently according to the strategies outlined in §2.1. To this end, we differentiate between the *desired* linear system $Mx = b$ and the *actual* linear system $\bar{M}\bar{x} = b$. Since IDALS updates the SUNMATRIX object infrequently, it is likely that $\alpha \neq \bar{\alpha}$, and in turn $M \neq \bar{M}$. 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 correct the linear system solution x via

$$x = \frac{2}{1+\alpha/\bar{\alpha}}\bar{x}. \tag{9.3}$$

The motivation for this selection of the scaling factor $c = 2/(1+\alpha/\bar{\alpha})$ is discussed in detail in [11, 31]. In short, if we consider a stationary iteration for the linear system as consisting of a solve with $\bar{M}$ followed by scaling by c, then for a linear constant-coefficient problem, the error in the solution vector will be reduced at each iteration by the error matrix $E = I - c\bar{M}^{-1}M$, with a convergence rate given by the spectral radius of E. Assuming that stiff systems have a spectrum spread widely over the left half-plane, c is chosen to minimize the magnitude of the eigenvalues of E.

9.4.2 Iterative linear solver tolerance

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE` then IDALS will set the input tolerance `delta` as described in §2.1. However, if the iterative linear solver does not support scaling matrices (i.e., the `SUNLinSolSetScalingVectors` routine is `NULL`), then IDALS will attempt to adjust the linear solver tolerance to account for this lack of functionality. To this end, the following assumptions are made:

1. All solution components have similar magnitude; hence the error weight vector W used in the

WRMS norm (see §2.1) should satisfy the assumption

$$W_i \approx W_{mean}, \quad \text{for} \quad i = 0, \ldots, n-1.$$

2. The SUNLINSOL object uses a standard 2-norm to measure convergence.

Since IDA uses identical left and right scaling matrices, $S_1 = S_2 = S = \text{diag}(W)$, then the linear solver convergence requirement is converted as follows (using the notation from equations (9.1)-(9.2)):

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

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2 / \sqrt{n}$$

is computed and the scaled tolerance `delta`$= \text{tol}/W_{mean}$ is supplied to the SUNLINSOL object.

9.5 The SUNLinearSolver_Dense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems. The SUNLINSOL_DENSE module is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_DENSE module, include the header file `sunlinsol/sunlinsol_dense.h`. We note that the SUNLINSOL_DENSE module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsoldense` module library.

9.5.1 SUNLinearSolver_Dense description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

9.5.2 SUNLinearSolver_Dense functions

The SUNLINSOL_DENSE module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

SUNLinSol_Dense	
Call	`LS = SUNLinSol_Dense(y, A);`
Description	The function `SUNLinSol_Dense` creates and allocates memory for a dense `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function `SUNDenseLinearSolver` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_Dense`

The SUNLINSOL_DENSE module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_Dense`
- `SUNLinSolInitialize_Dense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_Dense` – this performs the *LU* factorization.
- `SUNLinSolSolve_Dense` – this uses the *LU* factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_Dense`
- `SUNLinSolSpace_Dense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_Dense`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

9.5.3 SUNLinearSolver_Dense Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_DENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNDENSELINSOLINIT`

Call `FSUNDENSELINSOLINIT(code, ier)`

Description The function `FSUNDENSELINSOLINIT` can be called for Fortran programs to create a dense `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_DENSE module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSDENSELINSOLINIT`

Call `FSUNMASSDENSELINSOLINIT(ier)`

Description The function `FSUNMASSDENSELINSOLINIT` can be called for Fortran programs to create a dense `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.5.4 SUNLinearSolver_Dense content

The SUNLINSOL_DENSE module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Dense {
  sunindextype N;
  sunindextype *pivots;
  sunindextype last_flag;
};
```

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

`N` - size of the linear system,

`pivots` - index array for partial pivoting in LU factorization,

`last_flag` - last error return flag from internal function evaluations.

9.6 The SUNLinearSolver_Band implementation

This section describes the SUNLINSOL implementation for solving banded linear systems. The SUNLINSOL_BAND module is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_BAND module, include the header file `sunlinsol/sunlinsol_band.h`. We note that the SUNLINSOL_BAND module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolband` module library.

9.6.1 SUNLinearSolver_Band description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_BAND object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `ml`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1,mu+ml)`. The lower triangular factor L has lower bandwidth `ml`.

9.6.2 SUNLinearSolver_Band functions

The SUNLINSOL_BAND module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_Band`

Call	`LS = SUNLinSol_Band(y, A);`
Description	The function `SUNLinSol_Band` creates and allocates memory for a band `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_BAND matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check. Additionally, this routine will verify that the input matrix `A` is allocated with appropriate upper bandwidth storage for the LU factorization.
Deprecated Name	For backward compatibility, the wrapper function `SUNBandLinearSolver` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_Band`

The SUNLINSOL_BAND module defines band implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_Band`
- `SUNLinSolInitialize_Band` – this does nothing, since all consistency checks are performed at solver creation.

- SUNLinSolSetup_Band – this performs the LU factorization.
- SUNLinSolSolve_Band – this uses the LU factors and pivots array to perform the solve.
- SUNLinSolLastFlag_Band
- SUNLinSolSpace_Band – this only returns information for the storage *within* the solver object, i.e. storage for N, last_flag, and pivots.
- SUNLinSolFree_Band

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

9.6.3 SUNLinearSolver_Band Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_BAND module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNBANDLINSOLINIT

Call FSUNBANDLINSOLINIT(code, ier)

Description The function FSUNBANDLINSOLINIT can be called for Fortran programs to create a band SUNLinearSolver object.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value ier is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_BAND module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

`FSUNMASSBANDLINSOLINIT`

Call	`FSUNMASSBANDLINSOLINIT(ier)`
Description	The function `FSUNMASSBANDLINSOLINIT` can be called for Fortran programs to create a band `SUNLinearSolver` object for mass matrix linear systems.
Arguments	None
Return value	`ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.
Notes	This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.6.4 SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Band {
  sunindextype N;
  sunindextype *pivots;
  sunindextype last_flag;
};
```

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

`N` - size of the linear system,

`pivots` - index array for partial pivoting in LU factorization,

`last_flag` - last error return flag from internal function evaluations.

9.7 The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LAPACK. The SUNLINSOL_LAPACKDENSE module is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKDENSE module, include the header file `sunlinsol/sunlinsol_lapackdense.h`. The installed module library to link to is `libsundials_sunlinsollapackdense.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_LAPACKDENSE module is a SUNLINSOL wrapper for the LAPACK dense matrix factorization and solve routines, `*GETRF` and `*GETRS`, where `*` is either `D` or `S`, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKDENSE module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKDENSE module also cannot be compiled when using 64-bit integers for the `sunindextype`.

9.7.1 SUNLinearSolver_LapackDense description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.
- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

9.7.2 SUNLinearSolver_LapackDense functions

The SUNLINSOL_LAPACKDENSE module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_LapackDense`

Call	`LS = SUNLinSol_LapackDense(y, A);`
Description	The function `SUNLinSol_LapackDense` creates and allocates memory for a LAPACK-based, dense `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function `SUNLapackDense` with idential input and output arguments is also provided.

The SUNLINSOL_LAPACKDENSE module defines dense implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_LapackDense`
- `SUNLinSolInitialize_LapackDense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_LapackDense` – this calls either `DGETRF` or `SGETRF` to perform the LU factorization.
- `SUNLinSolSolve_LapackDense` – this calls either `DGETRS` or `SGETRS` to use the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_LapackDense`
- `SUNLinSolSpace_LapackDense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_LapackDense`

9.7.3 SUNLinearSolver_LapackDense Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKDENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNLAPACKDENSEINIT`

Call `FSUNLAPACKDENSEINIT(code, ier)`

Description The function `FSUNLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based dense `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKDENSE module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSLAPACKDENSEINIT`

Call `FSUNMASSLAPACKDENSEINIT(ier)`

Description The function `FSUNMASSLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based, dense `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.7.4 SUNLinearSolver_LapackDense content

The SUNLINSOL_LAPACKDENSE module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Dense {
  sunindextype N;
  sunindextype *pivots;
  sunindextype last_flag;
};
```

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

`N` - size of the linear system,

`pivots` - index array for partial pivoting in LU factorization,

`last_flag` - last error return flag from internal function evaluations.

9.8 The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LAPACK. The SUNLINSOL_LAPACKBAND module is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKBAND module, include the header file `sunlinsol/sunlinsol_lapackband.h`. The installed module library to link to is `libsundials_sunlinsollapackband.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_LAPACKBAND module is a SUNLINSOL wrapper for the LAPACK band matrix factorization and solve routines, *GBTRF and *GBTRS, where * is either D or S, depending on whether SUNDIALS was configured to have realtype set to double or single, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKBAND module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using extended precision for realtype. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKBAND module also cannot be compiled when using 64-bit integers for the sunindextype.

9.8.1 SUNLinearSolver_LapackBand description

This solver is constructed to perform the following operations:

- The "setup" call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the pivots array.
- The "solve" call performs pivoting and forward and backward substitution using the stored pivots array and the LU factors held in the SUNMATRIX_BAND object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth mu and lower bandwidth ml, then the upper triangular factor U can have upper bandwidth as big as smu = MIN(N-1,mu+ml). The lower triangular factor L has lower bandwidth ml.

9.8.2 SUNLinearSolver_LapackBand functions

The SUNLINSOL_LAPACKBAND module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_LapackBand

Call	LS = SUNLinSol_LapackBand(y, A);
Description	The function SUNLinSol_LapackBand creates and allocates memory for a LAPACK-based, band SUNLinearSolver object.
Arguments	y (N_Vector) a template for cloning vectors needed within the solver A (SUNMatrix) a SUNMATRIX_BAND matrix template for cloning matrices needed within the solver
Return value	This returns a SUNLinearSolver object. If either A or y are incompatible then this routine will return NULL.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check. Additionally, this routine will verify that the input matrix A is allocated with appropriate upper bandwidth storage for the LU factorization.
Deprecated Name	For backward compatibility, the wrapper function SUNLapackBand with idential input and output arguments is also provided.

The SUNLINSOL_LAPACKBAND module defines band implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_LapackBand`
- `SUNLinSolInitialize_LapackBand` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_LapackBand` – this calls either `DGBTRF` or `SGBTRF` to perform the *LU* factorization.
- `SUNLinSolSolve_LapackBand` – this calls either `DGBTRS` or `SGBTRS` to use the *LU* factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_LapackBand`
- `SUNLinSolSpace_LapackBand` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_LapackBand`

9.8.3 SUNLinearSolver_LapackBand Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKBAND module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNLAPACKDENSEINIT`

Call `FSUNLAPACKBANDINIT(code, ier)`

Description The function `FSUNLAPACKBANDINIT` can be called for Fortran programs to create a LAPACK-based band `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKBAND module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSLAPACKBANDINIT`

Call `FSUNMASSLAPACKBANDINIT(ier)`

Description The function `FSUNMASSLAPACKBANDINIT` can be called for Fortran programs to create a LAPACK-based, band `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

9.8.4 SUNLinearSolver_LapackBand content

The SUNLINSOL_LAPACKBAND module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Band {
  sunindextype N;
  sunindextype *pivots;
  sunindextype last_flag;
};
```

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

`N` - size of the linear system,

`pivots` - index array for partial pivoting in LU factorization,

`last_flag` - last error return flag from internal function evaluations.

9.9 The SUNLinearSolver_KLU implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with KLU. The SUNLINSOL_KLU module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

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

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [3, 22]. In order to use the SUNLINSOL_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to either `extended` or `single` (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available `sunindextype` options.

9.9.1 SUNLinearSolver_KLU description

The KLU library has a symbolic factorization routine that computes the permutation of the linear system matrix to block triangular form and the permutations that will pre-order the diagonal blocks (the only ones that need to be factored) to reduce fill-in (using AMD, COLAMD, CHOLAMD, natural, or an ordering given by the user). Of these ordering choices, the default value in the SUNLINSOL_KLU module is the COLAMD ordering.

KLU breaks the factorization into two separate parts. The first is a symbolic factorization and the second is a numeric factorization that returns the factored matrix along with final pivot information. KLU also has a refactor routine that can be called instead of the numeric factorization. This routine will reuse the pivot information. This routine also returns diagnostic information that a user can examine to determine if numerical stability is being lost and a full numerical factorization should be done instead of the refactor.

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

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.

- On subsequent calls to the "setup" routine, it calls the appropriate KLU "refactor" routine, followed by estimates of the numerical conditioning using the relevant "rcond", and if necessary "condest", routine(s). If these estimates of the condition number are larger than $\varepsilon^{-2/3}$ (where ε is the double-precision unit roundoff), then a new factorization is performed.
- The module includes the routine `SUNKLUReInit`, that can be called by the user to force a full or partial refactorization at the next "setup" call.
- The "solve" call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

9.9.2 SUNLinearSolver_KLU functions

The SUNLINSOL_KLU module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_KLU`

Call	`LS = SUNLinSol_KLU(y, A);`
Description	The function `SUNLinSol_KLU` creates and allocates memory for a KLU-based `SUNLinearSolver` object.
Arguments	`y` (`N_Vector`) a template for cloning vectors needed within the solver `A` (`SUNMatrix`) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
Return value	This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.
Notes	This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function `SUNKLU` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_KLU`

The SUNLINSOL_KLU module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_KLU`
- `SUNLinSolInitialize_KLU` – this sets the `first_factorize` flag to 1, forcing both symbolic and numerical factorizations on the subsequent "setup" call.
- `SUNLinSolSetup_KLU` – this performs either a *LU* factorization or refactorization of the input matrix.
- `SUNLinSolSolve_KLU` – this calls the appropriate KLU solve routine to utilize the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_KLU`
- `SUNLinSolSpace_KLU` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the KLU documentation.

- SUNLinSolFree_KLU

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_KLU module also defines the following additional user-callable functions.

SUNLinSol_KLUReInit

Call `retval = SUNLinSol_KLUReInit(LS, A, nnz, reinit_type);`

Description The function SUNLinSol_KLUReInit reinitializes memory and flags for a new factorization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed or if the structure of the linear system has changed which would require a new symbolic (and numeric factorization).

Arguments

LS	(SUNLinearSolver) a template for cloning vectors needed within the solver
A	(SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
nnz	(sunindextype) the new number of nonzeros in the matrix
reinit_type	(int) flag governing the level of reinitialization. The allowed values are:

- SUNKLU_REINIT_FULL – The Jacobian matrix will be destroyed and a new one will be allocated based on the nnz value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.
- SUNKLU_REINIT_PARTIAL – Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of nnz given in the sparse matrix provided to the original constructor routine (or the previous SUNLinSol_KLUReInit call).

Return value The return values from this function are SUNLS_MEM_NULL (either S or A are NULL), SUNLS_ILL_INPUT (A does not have type SUNMATRIX_SPARSE or reinit_type is invalid), SUNLS_MEM_FAIL (reallocation of the sparse matrix failed) or SUNLS_SUCCESS.

Notes This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

This routine assumes no other changes to solver use are necessary.

Deprecated Name For backward compatibility, the wrapper function SUNKLUReInit with idential input and output arguments is also provided.

F2003 Name FSUNLinSol_KLUReInit

SUNLinSol_KLUSetOrdering

Call `retval = SUNLinSol_KLUSetOrdering(LS, ordering);`

Description This function sets the ordering used by KLU for reducing fill in the linear solve.

Arguments

LS	(SUNLinearSolver) the SUNLINSOL_KLU object
ordering	(int) flag indicating the reordering algorithm to use, the options are:

0 AMD,

1 COLAMD, and
2 the natural ordering.

The default is 1 for COLAMD.

Return value The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid ordering choice), or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNKLUSetOrdering` with idential input and output arguments is also provided.

F2003 Name `FSUNLinSol_KLUSetOrdering`

`SUNLinSol_KLUGetSymbolic`

Call `symbolic = SUNLinSol_KLUGetSymbolic(LS);`

Description This function returns a pointer to the KLU symbolic factorization stored in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_symbolic`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_symbolic` is mapped to the KLU type `klu_symbolic`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`) this is mapped to the KLU type `klu_l_symbolic`.

`SUNLinSol_KLUGetNumeric`

Call `numeric = SUNLinSol_KLUGetNumeric(LS);`

Description This function returns a pointer to the KLU numeric factorization stored in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_numeric`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_numeric` is mapped to the KLU type `klu_numeric`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`), this is mapped to the KLU type `klu_l_numeric`.

`SUNLinSol_KLUGetCommon`

Call `common = SUNLinSol_KLUGetCommon(LS);`

Description This function returns a pointer to the KLU common structure stored within in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_common`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_common` is mapped to the KLU type `klu_common`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`), this is mapped to the KLU type `klu_l_common`.

9.9.3 SUNLinearSolver_KLU Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_KLU module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNKLUINIT`

Call `FSUNKLUINIT(code, ier)`

Description The function `FSUNKLUINIT` can be called for Fortran programs to create a SUNLINSOL_KLU object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_KLU module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSKLUINIT`

Call `FSUNMASSKLUINIT(ier)`

Description The function `FSUNMASSKLUINIT` can be called for Fortran programs to create a KLU-based `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

The `SUNLinSol_KLUReInit` and `SUNLinSol_KLUSetOrdering` routines also support FORTRAN interfaces for the system and mass matrix solvers:

`FSUNKLUREINIT`

Call `FSUNKLUREINIT(code, nnz, reinit_type, ier)`

Description The function `FSUNKLUREINIT` can be called for Fortran programs to re-initialize a SUNLINSOL_KLU object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`nnz` (`sunindextype*`) the new number of nonzeros in the matrix

`reinit_type` (`int*`) flag governing the level of reinitialization. The allowed values are:

1 – The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.

2 – Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the sparse matrix provided to the original constructor routine (or the previous `SUNLinSol_KLUReInit` call).

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUReInit` for complete further documentation of this routine.

`FSUNMASSKLUREINIT`

Call `FSUNMASSKLUREINIT(nnz, reinit_type, ier)`

Description The function `FSUNMASSKLUREINIT` can be called for Fortran programs to re-initialize a SUNLINSOL_KLU object for mass matrix linear systems.

Arguments The arguments are identical to `FSUNKLUREINIT` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUReInit` for complete further documentation of this routine.

`FSUNKLUSETORDERING`

Call `FSUNKLUSETORDERING(code, ordering, ier)`

Description The function `FSUNKLUSETORDERING` can be called for Fortran programs to change the reordering algorithm used by KLU.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`ordering` (`int*`) flag indication the reordering algorithm to use. Options include:

0 AMD,

1 COLAMD, and

2 the natural ordering.

The default is 1 for COLAMD.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUSetOrdering` for complete further documentation of this routine.

`FSUNMASSKLUSETORDERING`

Call `FSUNMASSKLUSETORDERING(ier)`

Description The function `FSUNMASSKLUSETORDERING` can be called for Fortran programs to change the reordering algorithm used by KLU for mass matrix linear systems.

Arguments The arguments are identical to `FSUNKLUSETORDERING` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_KLUSetOrdering` for complete further documentation of this routine.

9.9.4 SUNLinearSolver_KLU content

The SUNLINSOL_KLU module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_KLU {
  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, with underlying type `klu_symbolic` or `klu_l_symbolic`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively,

`numeric` - KLU storage structure for numeric factorization components, with underlying type `klu_numeric` or `klu_l_numeric`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively.

`common` - storage structure for common KLU solver components, with underlying type `klu_common` or `klu_l_common`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively,

`klu_solver` – pointer to the appropriate KLU solver function (depending on whether it is using a CSR or CSC sparse matrix, and on whether SUNDIALS was installed with 32-bit or 64-bit indices).

9.10 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.

9.10.1 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 [8, 28, 40, 41]. 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.

Starting with SuperLU_DIST version 6.3.0, some structures were renamed to have a prefix for the floating point type. The double precision API functions have the prefix 'd'. To maintain backwards compatibility with the unprefixed types, SUNDIALS provides macros to these SuperLU_DIST types with an 'x' prefix that expand to the correct prefix. E.g., the SUNDIALS macro `xLUstruct_t` expands to `dLUstruct_t` or `LUstruct_t` based on the SuperLU_DIST version.

9.10.2 SUNLinearSolver_SuperLUDIST functions

The SUNLINSOL_SUPERLUDIST module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1-9.1.3:

- `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 SUNLINSOL_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 SUNLINSOL_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 structure 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 structure 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 structure 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 structure that stores information about runtime and flop count.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `SuperLUStat_t*`

Notes

9.10.3 SUNLinearSolver_SuperLUDIST content

The SUNLINSOL_SUPERLUDIST module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SuperLUDIST {
  booleantype             first_factorize;
  int                     last_flag;
  realtype                berr;
  gridinfo_t              *grid;
  xLUstruct_t             *lu;
  superlu_dist_options_t  *options;
  xScalePermstruct_t      *scaleperm;
  xSOLVEstruct_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 transformations 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

9.11 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 [9, 39, 24]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step. In order to use the SUNLINSOL_SUPERLUMT interface to SUPERLUMT, it is assumed that SUPERLUMT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SUPERLUMT

(see Appendix A for details). Additionally, this wrapper only supports single- and double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to `extended` (see Section 4.2). Moreover, since the SUPERLUMT library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SUPERLUMT library is installed using the same integer precision as the SUNDIALS `sunindextype` option.

9.11.1 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.

9.11.2 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 9.1.1 – 9.1.3:

- `SUNLinSolGetType_SuperLUMT`
- `SUNLinSolInitialize_SuperLUMT` – this sets the `first_factorize` flag to 1 and resets the internal SUPERLUMT statistics variables.
- `SUNLinSolSetup_SuperLUMT` – this performs either a *LU* factorization or refactorization of the input matrix.
- `SUNLinSolSolve_SuperLUMT` – this calls the appropriate SUPERLUMT solve routine to utilize the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_SuperLUMT`
- `SUNLinSolSpace_SuperLUMT` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SUPERLUMT documentation.
- `SUNLinSolFree_SuperLUMT`

The SUNLINSOL_SUPERLUMT module also defines the following additional user-callable function.

`SUNLinSol_SuperLUMTSetOrdering`

Call `retval = SUNLinSol_SuperLUMTSetOrdering(LS, ordering);`

Description This function sets the ordering used by SUPERLUMT for reducing fill in the linear solve.

Arguments
- `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUMT object
- `ordering` (`int`) a flag indicating the ordering algorithm to use, the options are:
  - 0 natural ordering
  - 1 minimal degree ordering on $A^T A$
  - 2 minimal degree ordering on $A^T + A$
  - 3 COLAMD ordering for unsymmetric matrices

  The default is 3 for COLAMD.

Return value The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid ordering choice), or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSuperLUMTSetOrdering` with idential input and output arguments is also provided.

9.11.3 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 SUNLINSOL_KLU object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`num_threads` (`int*`) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SUPERLUMT module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSUPERLUMTINIT`

Call `FSUNMASSSUPERLUMTINIT(num_threads, ier)`

Description The function `FSUNMASSSUPERLUMTINIT` can be called for Fortran programs to create a SuperLU_MT-based `SUNLinearSolver` object for mass matrix linear systems.

Arguments `num_threads` (`int*`) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

The `SUNLinSol_SuperLUMTSetOrdering` routine also supports Fortran interfaces for the system and mass matrix solvers:

`FSUNSUPERLUMTSETORDERING`

Call `FSUNSUPERLUMTSETORDERING(code, ordering, ier)`

Description The function `FSUNSUPERLUMTSETORDERING` can be called for Fortran programs to update the ordering algorithm in a SUNLINSOL_SUPERLUMT object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`ordering` (`int*`) a flag indicating the ordering algorithm, options are:

- 0 natural ordering
- 1 minimal degree ordering on $A^T A$
- 2 minimal degree ordering on $A^T + A$
- 3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SuperLUMTSetOrdering` for complete further documentation of this routine.

`FSUNMASSUPERLUMTSETORDERING`

Call `FSUNMASSUPERLUMTSETORDERING(ordering, ier)`

Description The function `FSUNMASSUPERLUMTSETORDERING` can be called for Fortran programs to update the ordering algorithm in a SUNLINSOL_SUPERLUMT object for mass matrix linear systems.

Arguments `ordering` (`int*`) a flag indicating the ordering algorithm, options are:

- 0 natural ordering

1 minimal degree ordering on $A^T A$
2 minimal degree ordering on $A^T + A$
3 COLAMD ordering for unsymmetric matrices

The default is 3 for COLAMD.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SuperLUMTSetOrdering` for complete further documentation of this routine.

9.11.4 SUNLinearSolver_SuperLUMT content

The SUNLINSOL_SUPERLUMT module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_SuperLUMT {
  int          last_flag;
  int          first_factorize;
  SuperMatrix  *A, *AC, *L, *U, *B;
  Gstat_t      *Gstat;
  sunindextype *perm_r, *perm_c;
  sunindextype N;
  int          num_threads;
  realtype     diag_pivot_thresh;
  int          ordering;
  superlumt_options_t *options;
};
```

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

`last_flag` - last error return flag from internal function evaluations,

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

`A, AC, L, U, B` - `SuperMatrix` pointers used in solve,

`Gstat` - `GStat_t` object used in solve,

`perm_r, perm_c` - permutation arrays used in solve,

`N` - size of the linear system,

`num_threads` - number of OpenMP/Pthreads threads to use,

`diag_pivot_thresh` - threshold on diagonal pivoting,

`ordering` - flag for which reordering algorithm to use,

`options` - pointer to SUPERLUMT options structure.

9.12 The SUNLinearSolver_cuSolverSp_batchQR implementation

The `SUNLinearSolver_cuSolverSp_batchQR` implementation of the SUNLINSOL API is designed to be used with the `SUNMATRIX_CUSPARSE` matrix, and the NVECTOR_CUDA vector. The header file to include when using this module is `sunlinsol/sunlinsol_cusolversp_batchqr.h`. The installed library to link to is `libsundials_sunlinsolcusolversp.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The `SUNLinearSolver_cuSolverSp_batchQR` module is experimental and subject to change.

9.12.1 SUNLinearSolver_cuSolverSp_batchQR description

The SUNLinearSolver_cuSolverSp_batchQR implementation provides an interface to the batched sparse QR factorization method provided by the NVIDIA cuSOLVER library [6]. The module is designed for solving block diagonal linear systems of the form

$$\begin{bmatrix} \mathbf{A_1} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_n} \end{bmatrix} x_j = b_j$$

where all block matrices $\mathbf{A_j}$ share the same sparsisty pattern. The matrix must be the SUNMATRIX_CUSPARSE module.

9.12.2 SUNLinearSolver_cuSolverSp_batchQR functions

The SUNLinearSolver_cuSolverSp_batchQR module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1-9.1.3:

- SUNLinSolGetType_cuSolverSp_batchQR
- SUNLinSolInitialize_cuSolverSp_batchQR – this sets the first_factorize flag to 1
- SUNLinSolSetup_cuSolverSp_batchQR – this always copies the relevant SUNMATRIX_SPARSE data to the GPU; if this is the first setup it will perform symbolic analysis on the system
- SUNLinSolSolve_cuSolverSp_batchQR – this calls the cusolverSpXcsrqrsvBatched routine to perform factorization
- SUNLinSolLastFlag_cuSolverSp_batchQR
- SUNLinSolFree_cuSolverSp_batchQR

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

SUNLinSol_cuSolverSp_batchQR

Call `LS = SUNLinSol_cuSolverSp_batchQR(y, A, cusol);`

Description The function SUNLinSol_cuSolverSp_batchQR creates and allocates memory for a SUNLINSOL object.

Arguments

	y	(N_Vector) a NVECTOR_CUDA vector for checking compatibility with the solver
	A	(SUNMatrix) a SUNMATRIX_SPARSE matrix for checking compatibility with the solver
	cusol	(cusolverHandle_t) a valid cuSOLVER handle

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 solver.

This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMAT_CUSPARSE matrix type and the NVECTOR_CUDA vector type. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

`SUNLinSol_cuSolverSp_batchQR_GetDescription`

Call `SUNLinSol_cuSolverSp_batchQR_GetDescription(LS, &desc);`

Description The function `SUNLinSol_cuSolverSp_batchQR_GetDescription` accesses the string description of the object (empty by default).

Arguments
- `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
- `desc` (`char **`) the string description of the linear solver

Return value None

`SUNLinSol_cuSolverSp_batchQR_SetDescription`

Call `SUNLinSol_cuSolverSp_batchQR_SetDescription(LS, desc);`

Description The function `SUNLinSol_cuSolverSp_batchQR_SetDescription` sets the string description of the object (empty by default).

Arguments
- `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
- `desc` (`const char *`) the string description of the linear solver

Return value None

`SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace`

Call `SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace(LS, cuSolverInternal, cuSolverWorkspace);`

Description The function `SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace` returns the cuSOLVER batch QR method internal buffer size, in bytes, in the argument `cuSolverInternal` and the cuSOLVER batch QR workspace buffer size, in bytes, in the agrument `cuSolverWorkspace`. The size of the internal buffer is proportional to the number of matrix blocks while the size of the workspace is almost independent of the number of blocks.

Arguments
- `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
- `cuSolverInternal` (`size_t *`) output – the size of the cuSOLVER internal buffer in bytes
- `cuSolverWorkspace` (`size_t *`) output – the size of the cuSOLVER workspace buffer in bytes

Return value None

9.12.3 SUNLinearSolver_cuSolverSp_batchQR content

The `SUNLinearSolver_cuSolverSp_batchQR` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_cuSolverSp_batchQR {
  int                 last_flag;          /* last return flag                                  */
  booleantype         first_factorize;    /* is this the first factorization?                  */
  size_t              internal_size;      /* size of cusolver internal buffer for Q and R      */
  size_t              workspace_size;     /* size of cusolver memory block for num. factorization */
  cusolverSpHandle_t  cusolver_handle;    /* cuSolverSp context                                */
  csrqrInfo_t         info;               /* opaque cusolver data structure                    */
  void*               workspace;          /* memory block used by cusolver                     */
  const char*         desc;               /* description of this linear solver                 */
};
```

9.13 The SUNLinearSolver_MagmaDense implementation

The SUNLinearSolver_MagmaDense implementation of the SUNLINSOL API is designed to be used with the SUNMATRIX_MAGMADENSE matrix, and a GPU-enabled vector. This implementation interfaces to the MAGMA () linear algebra library and can target NVIDIA's CUDA programming model or AMD's HIP programming model [45].

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

The SUNLinearSolver_MagmaDense module is experimental and subject to change.

9.13.1 SUNLinearSolver_MagmaDense description

The SUNLinearSolver_MagmaDense implementation provides an interface to the dense LU and dense batched LU methods in the MAGMA linear algebra library [4]. The batched LU methods are leveraged when solving block diagonal linear systems of the form

$$\begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix} x_j = b_j.$$

9.13.2 SUNLinearSolver_MagmaDense functions

The SUNLinearSolver_MagmaDense module defines implementations of all "direct" linear solver operations listed in Sections 9.1.1-9.1.3:

- SUNLinSolGetType_MagmaDense
- SUNLinSolInitialize_MagmaDense
- SUNLinSolSetup_MagmaDense
- SUNLinSolSolve_MagmaDense
- SUNLinSolLastFlag_MagmaDense
- SUNLinSolFree_MagmaDense

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

SUNLinSol_MagmaDense

Call `LS = SUNLinSol_MagmaDense(y, A);`

Description The function SUNLinSol_MagmaDense creates and allocates memory for a SUNLINSOL object.

Arguments `y` (N_Vector) a vector for checking compatibility with the solver
`A` (SUNMatrix) a SUNMATRIX_MAGMADENSE matrix for checking compatibility with 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 analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the solver.

SUNLinSol_MagmaDense_SetAsync	
Call	`SUNLinSol_MagmaDense_SetAsync(SUNLinearSolver LS, booleantype onoff);`
Description	The function `SUNLinSol_MagmaDense_SetAsync` can be used to toggle the linear solver between asynchronous and synchronous modes. In asynchronous mode, `SUNLinearSolver` operations are asynchronous with respect to the host. In synchronous mode, the host and GPU device are synchronized prior to the operation returning.
Arguments	`LS` (`SUNLinearSolver`) a `SUNLinSol_MagmaDense` object `onoff` (`booleantype`) set to 0 for synchronous mode, or 1 for asynchronous mode
Return value	None
Notes	The default is asynchronous mode.

9.13.3 SUNLinearSolver_MagmaDense content

The `SUNLinearSolver_MagmaDense` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_MagmaDense {
  int             last_flag;
  booleantype     async;
  sunindextype    N;
  SUNMemory       pivots;
  SUNMemory       pivotsarr;
  SUNMemory       dpivotsarr;
  SUNMemory       infoarr;
  SUNMemory       rhsarr;
  SUNMemoryHelper memhelp;
  magma_queue_t   q;
};
```

9.14 The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [44]) iterative linear solver. The SUNLINSOL_SPGMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). When using Classical Gram-Schmidt, the optional function `N_VDotProdMulti` may be supplied for increased efficiency.

To access the SUNLINSOL_SPGMR module, include the header file `sunlinsol/sunlinsol_spgmr.h`. We note that the SUNLINSOL_SPGMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspgmr` module library.

9.14.1 SUNLinearSolver_SPGMR description

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)

- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the GMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

9.14.2 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	FSUNLinSol_SPGMR

The SUNLINSOL_SPGMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- SUNLinSolGetType_SPGMR
- SUNLinSolInitialize_SPGMR
- SUNLinSolSetATimes_SPGMR
- SUNLinSolSetPreconditioner_SPGMR
- SUNLinSolSetScalingVectors_SPGMR

- SUNLinSolSetup_SPGMR
- SUNLinSolSolve_SPGMR
- SUNLinSolNumIters_SPGMR
- SUNLinSolResNorm_SPGMR
- SUNLinSolResid_SPGMR
- SUNLinSolLastFlag_SPGMR
- SUNLinSolSpace_SPGMR
- SUNLinSolFree_SPGMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPGMR module also defines the following additional user-callable functions.

`SUNLinSol_SPGMRSetPrecType`

Call	`retval = SUNLinSol_SPGMRSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPGMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPGMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPGMR object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPGMR`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPGMRSetPrecType` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_SPGMRSetPrecType`

`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	`FSUNLinSol_SPGMRSetGSType`

`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 `FSUNLinSol_SPGMRSetMaxRestarts`

`SUNLinSolSetInfoFile_SPGMR`

Call `retval = SUNLinSolSetInfoFile_SPGMR(LS, info_file);`

Description The function `SUNLinSolSetInfoFile_SPGMR` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetInfoFile_SPGMR`

`SUNLinSolSetPrintLevel_SPGMR`

Call `retval = SUNLinSolSetPrintLevel_SPGMR(NLS, print_level);`

Description The function `SUNLinSolSetPrintLevel_SPGMR` specifies the level of verbosity of the output.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `print_level` (`int`) flag indicating level of verbosity; must be one of:
  - 0, no information is printed (default)
  - 1, for each linear iteration the residual norm is printed

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option** `SUNDIALS_BUILD_WITH_MONITORING`**, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetPrintLevel_SPGMR`

9.14.3 SUNLinearSolver_SPGMR Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPGMRINIT`

Call `FSUNSPGMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPGMRINIT`

Call `FSUNMASSSPGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object for mass matrix linear systems.

Arguments `pretype` (`int*`) flag indicating desired preconditioning type

`maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

The `SUNLinSol_SPGMRSetPrecType`, `SUNLinSol_SPGMRSetGSType` and `SUNLinSol_SPGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPGMRSETGSTYPE`

Call `FSUNSPGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

`FSUNMASSSPGMRSETGSTYPE`

Call `FSUNMASSSPGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

`FSUNSPGMRSETPRECTYPE`

Call `FSUNSPGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

FSUNMASSSPGMRSETPRECTYPE

Call `FSUNMASSSPGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

FSUNSPGMRSETMAXRS

Call `FSUNSPGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

FSUNMASSSPGMRSETMAXRS

Call `FSUNMASSSPGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

9.14.4 SUNLinearSolver_SPGMR content

The SUNLINSOL_SPGMR module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_SPGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  int numiters;
  realtype resnorm;
  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;
  int      print_level;
  FILE*    info_file;
};
```

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 (`maxl` + 1) $\times$ `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.

`print_level` - controls the amount of information to be printed to the info file

`info_file` - the file where all informative (non-error) messages will be directed

9.15 The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [43]) iterative linear solver. The SUNLINSOL_SPFGMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). When using Classical Gram-Schmidt, the optional function `N_VDotProdMulti` may be supplied for increased efficiency. Unlike the other Krylov iterative linear solvers supplied with SUNDIALS, SPFGMR is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

To access the SUNLINSOL_SPFGMR module, include the header file `sunlinsol/sunlinsol_spfgmr.h`. We note that the SUNLINSOL_SPFGMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspfgmr` module library.

9.15.1 SUNLinearSolver_SPFGMR description

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPFGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

9.15.2 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 `FSUNLinSol_SPFGMR`

SUNSPFGMR The SUNLINSOL_SPFGMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_SPFGMR`
- `SUNLinSolInitialize_SPFGMR`
- `SUNLinSolSetATimes_SPFGMR`
- `SUNLinSolSetPreconditioner_SPFGMR`
- `SUNLinSolSetScalingVectors_SPFGMR`
- `SUNLinSolSetup_SPFGMR`
- `SUNLinSolSolve_SPFGMR`
- `SUNLinSolNumIters_SPFGMR`
- `SUNLinSolResNorm_SPFGMR`
- `SUNLinSolResid_SPFGMR`
- `SUNLinSolLastFlag_SPFGMR`
- `SUNLinSolSpace_SPFGMR`
- `SUNLinSolFree_SPFGMR`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPFGMR module also defines the following additional user-callable functions.

`SUNLinSol_SPFGMRSetPrecType`

Call `retval = SUNLinSol_SPFGMRSetPrecType(LS, pretype);`

Description The function `SUNLinSol_SPFGMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPFGMR object.

Arguments
`LS` (`SUNLinearSolver`) the SUNLINSOL_SPFGMR object to update
`pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPFGMR`.

Return value This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSPFGMRSetPrecType` with idential input and output arguments is also provided.

F2003 Name `FSUNLinSol_SPFGMRSetPrecType`

`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 `FSUNLinSol_SPFGMRSetGSType`

`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 `FSUNLinSol_SPFGMRSetMaxRestarts`

`SUNLinSolSetInfoFile_SPFGMR`

Call `retval = SUNLinSolSetInfoFile_SPFGMR(LS, info_file);`

Description The function `SUNLinSolSetInfoFile_SPFGMR` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is
- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetInfoFile_SPFGMR`

`SUNLinSolSetPrintLevel_SPFGMR`

Call `retval = SUNLinSolSetPrintLevel_SPFGMR(NLS, print_level);`

Description The function `SUNLinSolSetPrintLevel_SPFGMR` specifies the level of verbosity of the output.

Arguments `LS` (`SUNLinearSolver`) a SUNNONLINSOL object

`print_level` (`int`) flag indicating level of verbosity; must be one of:

- 0, no information is printed (default)
- 1, for each linear iteration the residual norm is printed

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetPrintLevel_SPFGMR`

9.15.3 SUNLinearSolver_SPFGMR Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPFGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNSPFGMRINIT

Call `FSUNSPFGMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPFGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

FSUNMASSSPFGMRINIT

Call `FSUNMASSSPFGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

The `SUNLinSol_SPFGMRSetPrecType`, `SUNLinSol_SPFGMRSetGSType` and `SUNLinSol_SPFGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNSPFGMRSETGSTYPE

Call `FSUNSPFGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

FSUNMASSSPFGMRSETGSTYPE

Call `FSUNMASSSPFGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

`FSUNSPFGMRSETPRECTYPE`

Call `FSUNSPFGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETPRECTYPE`

Call `FSUNMASSSPFGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNSPFGMRSETMAXRS`

Call `FSUNSPFGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETMAXRS`

Call `FSUNMASSSPFGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

9.15.4 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;
  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;
  int      print_level;
  FILE*    info_file;
};
```

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

`maxl` - number of FGMRES basis vectors to use (default is 5),

`pretype` - flag for type of preconditioning to employ (default is none),

`gstype` - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

`max_restarts` - number of FGMRES restarts to allow (default is 0),

`numiters` - number of iterations from the most-recent solve,

`resnorm` - final linear residual norm from the most-recent solve,

`last_flag` - last error return flag from an internal function,

`ATimes` - function pointer to perform Av product,

`ATData` - pointer to structure for `ATimes`,

`Psetup` - function pointer to preconditioner setup routine,

`Psolve` - function pointer to preconditioner solve routine,

`PData` - pointer to structure for `Psetup` and `Psolve`,

`s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

`V` - the array of Krylov basis vectors $v_1, \ldots, v_{\texttt{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

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

`Hes` - the $(\texttt{maxl}+1) \times \texttt{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`.,

`givens` - a length `2*maxl` array which represents the Givens rotation matrices that arise in the FGMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where

$$F_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & -s_i & & & \\ & & & s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix},$$

are represented in the `givens` vector as `givens[0]` $= c_0$, `givens[1]` $= s_0$, `givens[2]` $= c_1$, `givens[3]` $= s_1$, ... `givens[2j]` $= c_j$, `givens[2j+1]` $= s_j$.,

`xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

`yg` - a length `(maxl+1)` array of `realtype` values used to hold "short" vectors (e.g. y and g),

`vtemp` - temporary vector storage.

`print_level` - controls the amount of information to be printed to the info file

`info_file` - the file where all informative (non-error) messages will be directed

9.16 The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [46]) iterative linear solver. The SUNLINSOL_SPBCGS module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VDiv`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, SPBCGS requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_SPBCGS module, include the header file `sunlinsol/sunlinsol_spbcgs.h`. We note that the SUNLINSOL_SPBCGS module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspbcgs` module library.

9.16.1 SUNLinearSolver_SPBCGS description

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPBCGS to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the SPBCGS iteration is performed. This will include scaling and preconditioning if those options have been supplied.

9.16.2 SUNLinearSolver_SPBCGS functions

The SUNLINSOL_SPBCGS module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPBCGS

Call `LS = SUNLinSol_SPBCGS(y, pretype, maxl);`

Description The function SUNLinSol_SPBCGS creates and allocates memory for a SPBCGS SUNLinearSolver object.

Arguments
- `y` (N_Vector) a template for cloning vectors needed within the solver
- `pretype` (int) flag indicating the desired type of preconditioning, allowed values are:
  - PREC_NONE (0)
  - PREC_LEFT (1)
  - PREC_RIGHT (2)
  - PREC_BOTH (3)

  Any other integer input will result in the default (no preconditioning).
- `maxl` (int) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value This returns a SUNLinearSolver object. If either y is incompatible then this routine will return NULL.

Notes This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPBCGS object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

Deprecated Name For backward compatibility, the wrapper function SUNSPBCGS with idential input and output arguments is also provided.

F2003 Name FSUNLinSol_SPBCGS

The SUNLINSOL_SPBCGS module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- SUNLinSolGetType_SPBCGS
- SUNLinSolInitialize_SPBCGS
- SUNLinSolSetATimes_SPBCGS
- SUNLinSolSetPreconditioner_SPBCGS
- SUNLinSolSetScalingVectors_SPBCGS

- SUNLinSolSetup_SPBCGS
- SUNLinSolSolve_SPBCGS
- SUNLinSolNumIters_SPBCGS
- SUNLinSolResNorm_SPBCGS
- SUNLinSolResid_SPBCGS
- SUNLinSolLastFlag_SPBCGS
- SUNLinSolSpace_SPBCGS
- SUNLinSolFree_SPBCGS

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPBCGS module also defines the following additional user-callable functions.

`SUNLinSol_SPBCGSSetPrecType`

Call	`retval = SUNLinSol_SPBCGSSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPBCGSSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPBCGS object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPBCGS object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPBCGS`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPBCGSSetPrecType` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_SPBCGSSetPrecType`

`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	`FSUNLinSol_SPBCGSSetMaxl`

`SUNLinSolSetInfoFile_SPBCGS`

Call `retval = SUNLinSolSetInfoFile_SPBCGS(LS, info_file);`

Description The function `SUNLinSolSetInfoFile_SPBCGS` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetInfoFile_SPBCGS`

`SUNLinSolSetPrintLevel_SPBCGS`

Call `retval = SUNLinSolSetPrintLevel_SPBCGS(NLS, print_level);`

Description The function `SUNLinSolSetPrintLevel_SPBCGS` specifies the level of verbosity of the output.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `print_level` (`int`) flag indicating level of verbosity; must be one of:
  - 0, no information is printed (default)
  - 1, for each linear iteration the residual norm is printed

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetPrintLevel_SPBCGS`

9.16.3 SUNLinearSolver_SPBCGS Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPBCGS module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPBCGSINIT`

Call `FSUNSPBCGSINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPBCGSINIT` can be called for Fortran programs to create a SUNLINSOL_SPBCGS object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPBCGS`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPBCGS module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPBCGSINIT`

Call `FSUNMASSSPBCGSINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPBCGSINIT` can be called for Fortran programs to create a SUNLINSOL_SPBCGS object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPBCGS`.

The `SUNLinSol_SPBCGSSetPrecType` and `SUNLinSol_SPBCGSSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPBCGSSETPRECTYPE`

Call `FSUNSPBCGSSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPBCGSSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPBCGSSETPRECTYPE`

Call `FSUNMASSSPBCGSSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPBCGSSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPBCGSSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetPrecType` for complete further documentation of this routine.

`FSUNSPBCGSSETMAXL`

Call `FSUNSPBCGSSETMAXL(code, maxl, ier)`

Description The function `FSUNSPBCGSSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetMaxl` for complete further documentation of this routine.

`FSUNMASSSPBCGSSETMAXL`

Call `FSUNMASSSPBCGSSETMAXL(maxl, ier)`

Description The function `FSUNMASSSPBCGSSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPBCGSSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPBCGSSetMaxl` for complete further documentation of this routine.

9.16.4 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;
  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;
  int      print_level;
  FILE*    info_file;
};
```

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.

`print_level` - controls the amount of information to be printed to the info file

`info_file` - the file where all informative (non-error) messages will be directed

9.17 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [27]) iterative linear solver. The SUNLINSOL_SPTFQMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, SPTFQMR requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_SPTFQMR module, include the header file `sunlinsol/sunlinsol_sptfqmr.h`. We note that the SUNLINSOL_SPTFQMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolsptfqmr` module library.

9.17.1 SUNLinearSolver_SPTFQMR description

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_SPTFQMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the TFQMR iteration is performed. This will include scaling and preconditioning if those options have been supplied.

9.17.2 SUNLinearSolver_SPTFQMR functions

The SUNLINSOL_SPTFQMR module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

`SUNLinSol_SPTFQMR`

Call `LS = SUNLinSol_SPTFQMR(y, pretype, maxl);`

Description The function `SUNLinSol_SPTFQMR` creates and allocates memory for a SPTFQMR `SUNLinearSolver` object.

Arguments
- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values are:
  - `PREC_NONE` (0)
  - `PREC_LEFT` (1)
  - `PREC_RIGHT` (2)
  - `PREC_BOTH` (3)

  Any other integer input will result in the default (no preconditioning).
- `maxl` (`int`) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).

Return value: This returns a `SUNLinearSolver` object. If either `y` is incompatible then this routine will return `NULL`.

Notes: This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If `y` is incompatible, then this routine will return `NULL`.

We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPTFQMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

Deprecated Name: For backward compatibility, the wrapper function `SUNSPTFQMR` with idential input and output arguments is also provided.

F2003 Name: `FSUNLinSol_SPTFQMR`

The SUNLINSOL_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_SPTFQMR`
- `SUNLinSolInitialize_SPTFQMR`
- `SUNLinSolSetATimes_SPTFQMR`
- `SUNLinSolSetPreconditioner_SPTFQMR`
- `SUNLinSolSetScalingVectors_SPTFQMR`
- `SUNLinSolSetup_SPTFQMR`
- `SUNLinSolSolve_SPTFQMR`
- `SUNLinSolNumIters_SPTFQMR`
- `SUNLinSolResNorm_SPTFQMR`
- `SUNLinSolResid_SPTFQMR`
- `SUNLinSolLastFlag_SPTFQMR`
- `SUNLinSolSpace_SPTFQMR`
- `SUNLinSolFree_SPTFQMR`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPTFQMR module also defines the following additional user-callable functions.

`SUNLinSol_SPTFQMRSetPrecType`

Call: `retval = SUNLinSol_SPTFQMRSetPrecType(LS, pretype);`

Description: The function `SUNLinSol_SPTFQMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPTFQMR object.

Arguments:
- `LS` (`SUNLinearSolver`) the SUNLINSOL_SPTFQMR object to update
- `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPTFQMR`.

Return value: This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name: For backward compatibility, the wrapper function `SUNSPTFQMRSetPrecType` with idential input and output arguments is also provided.

F2003 Name: `FSUNLinSol_SPTFQMRSetPrecType`

`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 `FSUNLinSol_SPTFQMRSetMaxl`

SUNSPTFQMRSetMaxl

`SUNLinSolSetInfoFile_SPTFQMR`

Call `retval = SUNLinSolSetInfoFile_SPTFQMR(LS, info_file);`

Description The function `SUNLinSolSetInfoFile_SPTFQMR` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetInfoFile_SPTFQMR`

`SUNLinSolSetPrintLevel_SPTFQMR`

Call `retval = SUNLinSolSetPrintLevel_SPTFQMR(NLS, print_level);`

Description The function `SUNLinSolSetPrintLevel_SPTFQMR` specifies the level of verbosity of the output.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `print_level` (`int`) flag indicating level of verbosity; must be one of:
  - 0, no information is printed (default)
  - 1, for each linear iteration the residual norm is printed

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option** `SUNDIALS_BUILD_WITH_MONITORING`**, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetPrintLevel_SPTFQMR`

9.17.3 SUNLinearSolver_SPTFQMR Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPTFQMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPTFQMRINIT`

Call `FSUNSPTFQMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPTFQMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPTFQMRINIT`

Call `FSUNMASSSPTFQMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object for mass matrix linear systems.

Arguments `pretype` (`int*`) flag indicating desired preconditioning type
`maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

The `SUNLinSol_SPTFQMRSetPrecType` and `SUNLinSol_SPTFQMRSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPTFQMRSETPRECTYPE`

Call `FSUNSPTFQMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPTFQMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPTFQMRSETPRECTYPE`

Call `FSUNMASSSPTFQMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPTFQMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPTFQMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetPrecType` for complete further documentation of this routine.

`FSUNSPTFQMRSETMAXL`

Call `FSUNSPTFQMRSETMAXL(code, maxl, ier)`

Description The function `FSUNSPTFQMRSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetMaxl` for complete further documentation of this routine.

`FSUNMASSSPTFQMRSETMAXL`

Call `FSUNMASSSPTFQMRSETMAXL(maxl, ier)`

Description The function `FSUNMASSSPTFQMRSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPTFQMRSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPTFQMRSetMaxl` for complete further documentation of this routine.

9.17.4 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;
  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;
  int      print_level;
  FILE*    info_file;
};
```

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.

`print_level` - controls the amount of information to be printed to the info file

`info_file` - the file where all informative (non-error) messages will be directed

9.18 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementaiton of the PCG (Preconditioned Conjugate Gradient [29]) iterative linear solver. The SUNLINSOL_PCG module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, PCG requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_PCG module, include the header file `sunlinsol/sunlinsol_pcg.h`. We note that the SUNLINSOL_PCG module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolpcg` module library.

9.18.1 SUNLinearSolver_PCG description

Unlike all of the other iterative linear solvers supplied with SUNDIALS, PCG should only be used on *symmetric* linear systems (e.g. mass matrix linear systems encountered in ARKODE). As a result, the explanation of the role of scaling and preconditioning matrices given in general must be modified in this scenario. The PCG algorithm solves a linear system $Ax = b$ where A is a symmetric ($A^T = A$), real-valued matrix. Preconditioning is allowed, and is applied in a symmetric fashion on both the right and left. Scaling is also allowed and is applied symmetrically. We denote the preconditioner and scaling matrices as follows:

- P is the preconditioner (assumed symmetric),
- S is a diagonal matrix of scale factors.

The matrices A and P are not required explicitly; only routines that provide A and P^{-1} as operators are required. The diagonal of the matrix S is held in a single NVECTOR, supplied by the user.

In this notation, PCG applies the underlying CG algorithm to the equivalent transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.4}$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \tag{9.5}$$

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

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

where $\|v\|_S = \sqrt{v^T S^T S v}$, with an input tolerance δ.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_PCG to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s` scaling vector.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

9.18.2 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 `FSUNLinSol_PCG`

The SUNLINSOL_PCG module defines implementations of all "iterative" linear solver operations listed in Sections 9.1.1 – 9.1.3:

- `SUNLinSolGetType_PCG`
- `SUNLinSolInitialize_PCG`
- `SUNLinSolSetATimes_PCG`
- `SUNLinSolSetPreconditioner_PCG`
- `SUNLinSolSetScalingVectors_PCG` – since PCG only supports symmetric scaling, the second NVECTOR argument to this function is ignored
- `SUNLinSolSetup_PCG`
- `SUNLinSolSolve_PCG`
- `SUNLinSolNumIters_PCG`
- `SUNLinSolResNorm_PCG`
- `SUNLinSolResid_PCG`
- `SUNLinSolLastFlag_PCG`
- `SUNLinSolSpace_PCG`
- `SUNLinSolFree_PCG`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_PCG module also defines the following additional user-callable functions.

`SUNLinSol_PCGSetPrecType`

Call `retval = SUNLinSol_PCGSetPrecType(LS, pretype);`

Description The function `SUNLinSol_PCGSetPrecType` updates the flag indicating use of preconditioning in the SUNLINSOL_PCG object.

Arguments
- `LS` (`SUNLinearSolver`) the SUNLINSOL_PCG object to update
- `pretype` (`int`) flag indicating use of preconditioning, allowed values match those discussed in `SUNLinSol_PCG`.

Return value This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNPCGSetPrecType` with idential input and output arguments is also provided.

F2003 Name `FSUNLinSol_PCGSetPrecType`

`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 `FSUNLinSol_PCGSetMaxl`

`SUNLinSolSetInfoFile_PCG`

Call `retval = SUNLinSolSetInfoFile_PCG(LS, info_file);`

Description The function `SUNLinSolSetInfoFile_PCG` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetInfoFile_PCG`

`SUNLinSolSetPrintLevel_PCG`

Call `retval = SUNLinSolSetPrintLevel_PCG(NLS, print_level);`

Description The function `SUNLinSolSetPrintLevel_PCG` specifies the level of verbosity of the output.

Arguments
- `LS` (`SUNLinearSolver`) a SUNNONLINSOL object
- `print_level` (`int`) flag indicating level of verbosity; must be one of:
  - 0, no information is printed (default)
  - 1, for each linear iteration the residual norm is printed

Return value The return value is

- `SUNLS_SUCCESS` if successful
- `SUNLS_MEM_NULL` if the SUNLinearSolver memory was `NULL`
- `SUNLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option** `SUNDIALS_BUILD_WITH_MONITORING`**, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNLinSolSetPrintLevel_PCG`

9.18.3 SUNLinearSolver_PCG Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_PCG module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNPCGINIT`

Call `FSUNPCGINIT(code, pretype, maxl, ier)`

Description The function `FSUNPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_PCG module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSPCGINIT`

Call `FSUNMASSPCGINIT(pretype, maxl, ier)`

Description The function `FSUNMASSPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

The `SUNLinSol_PCGSetPrecType` and `SUNLinSol_PCGSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNPCGSETPRECTYPE`

Call `FSUNPCGSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNPCGSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetPrecType` for complete further documentation of this routine.

`FSUNMASSPCGSETPRECTYPE`

Call `FSUNMASSPCGSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSPCGSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNPCGSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetPrecType` for complete further documentation of this routine.

`FSUNPCGSETMAXL`

Call `FSUNPCGSETMAXL(code, maxl, ier)`

Description The function `FSUNPCGSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetMaxl` for complete further documentation of this routine.

`FSUNMASSPCGSETMAXL`

Call `FSUNMASSPCGSETMAXL(maxl, ier)`

Description The function `FSUNMASSPCGSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNPCGSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetMaxl` for complete further documentation of this routine.

9.18.4 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;
  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;
  int      print_level;
  FILE*    info_file;
};
```

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.

`print_level` - controls the amount of information to be printed to the info file

`info_file` - the file where all informative (non-error) messages will be directed

9.19 SUNLinearSolver Examples

There are `SUNLinearSolver` examples that may be installed for each implementation; these make use of the functions in `test_sunlinsol.c`. These example functions show simple usage of the

SUNLinearSolver family of functions. The inputs to the examples depend on the linear solver type, and are output to stdout if the example is run without the appropriate number of command-line arguments.
The following is a list of the example functions in test_sunlinsol.c:

- Test_SUNLinSolGetType: Verifies the returned solver type against the value that should be returned.
- Test_SUNLinSolInitialize: Verifies that SUNLinSolInitialize can be called and returns successfully.
- Test_SUNLinSolSetup: Verifies that SUNLinSolSetup can be called and returns successfully.
- Test_SUNLinSolSolve: Given a SUNMATRIX object A, NVECTOR objects x and b (where $Ax = b$) and a desired solution tolerance tol, this routine clones x into a new vector y, calls SUNLinSolSolve to fill y as the solution to $Ay = b$ (to the input tolerance), verifies that each entry in x and y match to within 10*tol, and overwrites x with y prior to returning (in case the calling routine would like to investigate further).
- Test_SUNLinSolSetATimes (iterative solvers only): Verifies that SUNLinSolSetATimes can be called and returns successfully.
- Test_SUNLinSolSetPreconditioner (iterative solvers only): Verifies that SUNLinSolSetPreconditioner can be called and returns successfully.
- Test_SUNLinSolSetScalingVectors (iterative solvers only): Verifies that SUNLinSolSetScalingVectors can be called and returns successfully.
- Test_SUNLinSolLastFlag: Verifies that SUNLinSolLastFlag can be called, and outputs the result to stdout.
- Test_SUNLinSolNumIters (iterative solvers only): Verifies that SUNLinSolNumIters can be called, and outputs the result to stdout.
- Test_SUNLinSolResNorm (iterative solvers only): Verifies that SUNLinSolResNorm can be called, and that the result is non-negative.
- Test_SUNLinSolResid (iterative solvers only): Verifies that SUNLinSolResid can be called.
- Test_SUNLinSolSpace verifies that SUNLinSolSpace can be called, and outputs the results to stdout.

We'll note that these tests should be performed in a particular order. For either direct or iterative linear solvers, Test_SUNLinSolInitialize must be called before Test_SUNLinSolSetup, which must be called before Test_SUNLinSolSolve. Additionally, for iterative linear solvers Test_SUNLinSolSetATimes, Test_SUNLinSolSetPreconditioner and Test_SUNLinSolSetScalingVectors should be called before Test_SUNLinSolInitialize; similarly Test_SUNLinSolNumIters, Test_SUNLinSolResNorm and Test_SUNLinSolResid should be called after Test_SUNLinSolSolve. These are called in the appropriate order in all of the example problems.

Chapter 10

Description of the SUNNonlinearSolver module

SUNDIALS time integration packages are written in terms of generic nonlinear solver operations defined by the SUNNONLINSOL API and implemented by a particular SUNNONLINSOL module of type `SUNNonlinearSolver`. Users can supply their own SUNNONLINSOL module, or use one of the modules provided with SUNDIALS. Depending on the package, nonlinear solver modules can either target system presented in a rootfinding ($F(y) = 0$) or fixed-point ($G(y) = y$) formulation. For more information on the formulation of the nonlinear system(s) see section 10.2.

The time integrators in SUNDIALS specify a default nonlinear solver module and as such this chapter is intended for users that wish to use a non-default nonlinear solver module or would like to provide their own nonlinear solver implementation. Users interested in using a non-default solver module may skip the description of the SUNNONLINSOL API in section 10.1 and proceeded to the subsequent sections in this chapter that describe the SUNNONLINSOL modules provided with SUNDIALS.

For users interested in providing their own SUNNONLINSOL module, the following section presents the SUNNONLINSOL API and its implementation beginning with the definition of SUNNONLINSOL functions in sections 10.1.1 – 10.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 10.1.4. A table of nonlinear solver return codes is given in section 10.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 10.1.6. Section 10.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 10.1.8 lists the requirements for supplying a custom SUNNONLINSOL module. Users wishing to supply their own SUNNONLINSOL module are encouraged to use the SUNNONLINSOL implementations provided with SUNDIALS as a template for supplying custom nonlinear solver modules.

10.1 The SUNNonlinearSolver API

The SUNNONLINSOL API defines several nonlinear solver operations that enable SUNDIALS integrators to utilize any SUNNONLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core nonlinear solver functions. The second group of functions consists of set routines to supply the nonlinear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving nonlinear solver statistics. All of these functions are defined in the header file `sundials/sundials_nonlinearsolver.h`.

10.1.1 SUNNonlinearSolver core functions

The core nonlinear solver functions consist of two required functions to get the nonlinear solver type (`SUNNonlinsSolGetType`) and solve the nonlinear system (`SUNNonlinSolSolve`). The remaining three

functions for nonlinear solver initialization (`SUNNonlinSolInitialization`), setup (`SUNNonlinSolSetup`), and destruction (`SUNNonlinSolFree`) are optional.

`SUNNonlinSolGetType`

Call `type = SUNNonlinSolGetType(NLS);`

Description The *required* function `SUNNonlinSolGetType` returns nonlinear solver type.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

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

`SUNNONLINEARSOLVER_ROOTFIND` `0`, the SUNNONLINSOL module solves $F(y) = 0$.

`SUNNONLINEARSOLVER_FIXEDPOINT` `1`, the SUNNONLINSOL module solves $G(y) = y$.

F2003 Name `FSUNNonlinSolGetType`

`SUNNonlinSolInitialize`

Call `retval = SUNNonlinSolInitialize(NLS);`

Description The *optional* function `SUNNonlinSolInitialize` performs nonlinear solver initialization and may perform any necessary memory allocations.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

Return value The return value `retval` (of type `int`) is zero for a successful call and a negative value for a failure.

Notes It is assumed all solver-specific options have been set prior to calling `SUNNonlinSolInitialize`. SUNNONLINSOL implementations that do not require initialization may set this operation to `NULL`.

F2003 Name `FSUNNonlinSolInitialize`

`SUNNonlinSolSetup`

Call `retval = SUNNonlinSolSetup(NLS, y, mem);`

Description The *optional* function `SUNNonlinSolSetup` performs any solver setup needed for a nonlinear solve.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

`y` (`N_Vector`) the initial iteration passed to the nonlinear solver.

`mem` (`void *`) the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successful call and a negative value for a failure.

Notes SUNDIALS integrators call `SUNonlinSolSetup` before each step attempt. SUNNONLINSOL implementations that do not require setup may set this operation to `NULL`.

F2003 Name `FSUNNonlinSolSetup`

`SUNNonlinSolSolve`

Call `retval = SUNNonlinSolSolve(NLS, y0, ycor, 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 predicted value for the new solution state. This *must* remain unchanged throughout the solution process. See section 10.2 for more detail on the nonlinear system formulation.

`ycor` (`N_Vector`) on input the initial guess for the correction to the predicted state (zero) and on output the final correction to the predicted state. See section 10.2 for more detail on the nonlinear system formulation.

`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 (i.e., the solve failed and the integrator should reduce the step size and reattempt the step), and a negative value for an unrecoverable error (i.e., the solve failed and the integrator should halt and return an error to the user).

F2003 Name `FSUNNonlinSolSolve`

`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`.

F2003 Name `FSUNNonlinSolFree`

10.1.2 SUNNonlinearSolver set functions

The following set functions are used to supply nonlinear solver modules with functions defined by the SUNDIALS integrators and to modify solver parameters. Only the routine for setting the nonlinear system defining function (`SUNNonlinSolSetSysFn` is required. All other set functions are optional.

`SUNNonlinSolSetSysFn`

Call `retval = SUNNonlinSolSetSysFn(NLS, SysFn);`

Description The *required* function `SUNNonlinSolSetSysFn` is used to provide the nonlinear solver with the function defining the nonlinear system. This is the function $F(y)$ in $F(y) = 0$ for `SUNNONLINEARSOLVER_ROOTFIND` modules or $G(y)$ in $G(y) = y$ for `SUNNONLINEARSOLVER_FIXEDPOINT` modules.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.

`SysFn` (`SUNNonlinSolSysFn`) the function defining the nonlinear system. See section 10.1.4 for the definition of `SUNNonlinSolSysFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolSetSysFn`

`SUNNonlinSolSetLSetupFn`

Call `retval = SUNNonlinSolSetLSetupFn(NLS, LSetupFn);`

Description The *optional* function `SUNNonlinSolLSetupFn` is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver setup function.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
- `LSetupFn` (`SUNNonlinSolLSetupFn`) a wrapper function to the SUNDIALS integrator's linear solver setup function. See section 10.1.4 for the definition of `SUNNonlinLSetupFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes The `SUNNonlinLSetupFn` function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLINSOL direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLINSOL iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize SUNLINSOL linear solvers, or use SUNLINSOL linear solvers that do not require setup may set this operation to `NULL`.

F2003 Name `FSUNNonlinSolSetLSetupFn`

`SUNNonlinSolSetLSolveFn`

Call `retval = SUNNonlinSolSetLSolveFn(NLS, LSolveFn);`

Description The *optional* function `SUNNonlinSolSetLSolveFn` is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver solve function.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
- `LSolveFn` (`SUNNonlinSolLSolveFn`) a wrapper function to the SUNDIALS integrator's linear solver solve function. See section 10.1.4 for the definition of `SUNNonlinSolLSolveFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes The `SUNNonlinLSolveFn` function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNONLINSOL implementations that do not require solving this system or do not use SUNLINSOL linear solvers may set this operation to `NULL`.

F2003 Name `FSUNNonlinSolSetLSolveFn`

`SUNNonlinSolSetConvTestFn`

Call `retval = SUNNonlinSolSetConvTestFn(NLS, CTestFn, ctest_data);`

Description The *optional* function `SUNNonlinSolSetConvTestFn` is used to provide the nonlinear solver with a function for determining if the nonlinear solver iteration has converged. This is typically called by SUNDIALS integrators to define their nonlinear convergence criteria, but may be replaced by the user.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
- `CTestFn` (`SUNNonlineSolConvTestFn`) a SUNDIALS integrator's nonlinear solver convergence test function. See section 10.1.4 for the definition of `SUNNonlinSolConvTestFn`.
- `ctest_data` (`void*`) is a data pointer passed to `CTestFn` every time it is called.

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`.

F2003 Name `FSUNNonlinSolSetConvTestFn`

`SUNNonlinSolSetMaxIters`

Call `retval = SUNNonlinSolSetMaxIters(NLS, maxiters);`

Description The *optional* function `SUNNonlinSolSetMaxIters` sets the maximum number of nonlinear solver iterations. This is typically called by SUNDIALS integrators to define their default iteration limit, but may be adjusted by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
`maxiters` (`int`) the maximum number of nonlinear iterations.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure (e.g., `maxiters` < 1).

F2003 Name `FSUNNonlinSolSetMaxIters`

10.1.3 SUNNonlinearSolver get functions

The following get functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routines to get number of iterations in the most recent solve (`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 number of nonlinear solver iterations in the most recent solve. 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.

F2003 Name `FSUNNonlinSolGetNumIters`

`SUNNonlinSolGetCurIter`

Call `retval = SUNNonlinSolGetCurIter(NLS, iter);`

Description The function `SUNNonlinSolGetCurIter` returns the iteration index of the current nonlinear solve. This function is *required* when using SUNDIALS integrator-provided convergence tests or when using a SUNLINSOL spils linear solver; otherwise it is *optional*.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`iter` (`int*`) the nonlinear solver iteration in the current solve starting from zero.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolGetCurIter`

`SUNNonlinSolGetNumConvFails`

Call `retval = SUNNonlinSolGetNumConvFails(NLS, nconvfails);`

Description The *optional* function `SUNNonlinSolGetNumConvFails` returns the number of nonlinear solver convergence failures in the most recent solve. 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
`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.

F2003 Name `FSUNNonlinSolGetNumConvFails`

10.1.4 Functions provided by SUNDIALS integrators

To interface with SUNNONLINSOL modules, the SUNDIALS integrators supply a variety of routines for evaluating the nonlinear system, calling the SUNLINSOL setup and solve functions, and testing the nonlinear iteration for convergence. These integrator-provided routines translate between the user-supplied ODE or DAE systems and the generic interfaces to the nonlinear or linear systems of equations that result in their solution. The types for functions provided to a SUNNONLINSOL module are defined in the header file `sundials/sundials_nonlinearsolver.h`, and are described below.

`SUNNonlinSolSysFn`

Definition `typedef int (*SUNNonlinSolSysFn)(N_Vector ycor, 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 `ycor` will be left unchanged.

Arguments `ycor` is the current correction to the predicted state at which the nonlinear system should be evaluated. See section 10.2 for more detail on the nonlinear system formulation.
`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.

Notes As discussed in section 10.2, SUNDIALS integrators formulate nonlinear systems as a function of the correction to the predicted solution. On each call to the nonlinear system function the integrator will compute and store the current solution based on the input correction. Additionally, the residual will store the value of the ODE right-hand side function or DAE residual used in computing the nonlinear system residual. These stored values are then directly used in the integrator-supplied linear solver setup and solve functions as applicable.

`SUNNonlinSolLSetupFn`

Definition `typedef int (*SUNNonlinSolLSetupFn)(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 `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.

As discussed in the description of `SUNNonlinSolSysFn`, the linear solver setup function assumes that the nonlinear system function has been called prior to the linear solver setup function as the setup will utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

`SUNNonlinSolLSolveFn`

Definition
```
typedef int (*SUNNonlinSolLSolveFn)(N_Vector b, void* mem);
```

Purpose These functions are wrappers to the SUNDIALS integrator's function for solving linear systems with SUNLINSOL modules.

Arguments `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.

As discussed in the description of `SUNNonlinSolSysFn`, the linear solver solve function assumes that the nonlinear system function has been called prior to the linear solver solve function as the solve may utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

`SUNNonlinSolConvTestFn`

Definition
```
typedef int (*SUNNonlinSolConvTestFn)(SUNNonlinearSolver NLS, N_Vector ycor,
                                      N_Vector del, realtype tol,
                                      N_Vector ewt, void* ctest_data);
```

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.
`ycor` is the current correction (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.
`ctest_data` is the data pointer provided to `SUNNonlinSolSetConvTestFn`.

Return value The return value of this routine will be a negative value if an unrecoverable error occurred or one of the following:

SUN_NLS_SUCCESS	the iteration is converged.
SUN_NLS_CONTINUE	the iteration has not converged, keep iterating.
SUN_NLS_CONV_RECVR	the iteration appears to be diverging, try to recover.

Notes The tolerance passed to this routine by SUNDIALS integrators is the tolerance in a weighted root-mean-squared norm with error weight vector `ewt`. SUNNONLINSOL modules utilizing their own convergence criteria may ignore these functions.

10.1.5 SUNNonlinearSolver return codes

The functions provided to SUNNONLINSOL modules by each SUNDIALS integrator, and functions within the SUNDIALS-provided SUNNONLINSOL implementations utilize a common set of return codes, shown below in Table 10.1. Here, negative values correspond to non-recoverable failures, positive values to recoverable failures, and zero to a successful call.

Table 10.1: Description of the `SUNNonlinearSolver` return codes

Name	Value	Description
SUN_NLS_SUCCESS	0	successful call or converged solve
SUN_NLS_CONTINUE	901	the nonlinear solver is not converged, keep iterating
SUN_NLS_CONV_RECVR	902	the nonlinear solver appears to be diverging, try to recover
SUN_NLS_MEM_NULL	-901	a memory argument is NULL
SUN_NLS_MEM_FAIL	-902	a memory access or allocation failed
SUN_NLS_ILL_INPUT	-903	an illegal input option was provided
SUN_NLS_VECTOROP_ERR	-904	a NVECTOR operation failed
SUN_NLS_EXT_FAIL	-905	an external library call returned an error

10.1.6 The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic SUNNONLINSOL module on which all other SUNNONLINSOL implementations are built. The `SUNNonlinearSolver` type is a pointer to a structure containing an implementation-dependent *content* field and an *ops* field. The type `SUNNonlinearSolver` is defined as follows:

```
typedef struct _generic_SUNNonlinearSolver *SUNNonlinearSolver;

struct _generic_SUNNonlinearSolver {
  void *content;
  struct _generic_SUNNonlinearSolver_Ops *ops;
};
```

where the `_generic_SUNNonlinearSolver_Ops` structure is a list of pointers to the various actual nonlinear solver operations provided by a specific implementation. The `_generic_SUNNonlinearSolver_Ops` structure is defined as

```
struct _generic_SUNNonlinearSolver_Ops {
  SUNNonlinearSolver_Type (*gettype)(SUNNonlinearSolver);
  int                     (*initialize)(SUNNonlinearSolver);
  int                     (*setup)(SUNNonlinearSolver, N_Vector, void*);
  int                     (*solve)(SUNNonlinearSolver, N_Vector, N_Vector,
                                   N_Vector, realtype, booleantype, void*);
```

```
  int                    (*free)(SUNNonlinearSolver);
  int                    (*setsysfn)(SUNNonlinearSolver, SUNNonlinSolSysFn);
  int                    (*setlsetupfn)(SUNNonlinearSolver, SUNNonlinSolLSetupFn);
  int                    (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
  int                    (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn,
                                       void*);
  int                    (*setmaxiters)(SUNNonlinearSolver, int);
  int                    (*getnumiters)(SUNNonlinearSolver, long int*);
  int                    (*getcuriter)(SUNNonlinearSolver, int*);
  int                    (*getnumconvfails)(SUNNonlinearSolver, long int*);
};
```

The generic SUNNONLINSOL module defines and implements the nonlinear solver operations defined in Sections 10.1.1 – 10.1.3. These routines are in fact only wrappers to the nonlinear solver operations provided by a particular SUNNONLINSOL implementation, which are accessed through the ops field of the `SUNNonlinearSolver` structure. To illustrate this point we show below the implementation of a typical nonlinear solver operation from the generic SUNNONLINSOL module, namely `SUNNonlinSolSolve`, which solves the nonlinear system and returns a flag denoting a successful or failed solve:

```
int SUNNonlinSolSolve(SUNNonlinearSolver NLS,
                      N_Vector y0, N_Vector y,
                      N_Vector w, realtype tol,
                      booleantype callLSetup, void* mem)
{
  return((int) NLS->ops->solve(NLS, y0, y, w, tol, callLSetup, mem));
}
```

The Fortran 2003 interface provides a `bind(C)` derived-type for the `_generic_SUNNonlinearSolver` and the `_generic_SUNNonlinearSolver_Ops` structures. Their definition is given below.

```
 type, bind(C), public :: SUNNonlinearSolver
  type(C_PTR), public :: content
  type(C_PTR), public :: ops
 end type SUNNonlinearSolver

 type, bind(C), public :: SUNNonlinearSolver_Ops
  type(C_FUNPTR), public :: gettype
  type(C_FUNPTR), public :: initialize
  type(C_FUNPTR), public :: setup
  type(C_FUNPTR), public :: solve
  type(C_FUNPTR), public :: free
  type(C_FUNPTR), public :: setsysfn
  type(C_FUNPTR), public :: setlsetupfn
  type(C_FUNPTR), public :: setlsolvefn
  type(C_FUNPTR), public :: setctestfn
  type(C_FUNPTR), public :: setmaxiters
  type(C_FUNPTR), public :: getnumiters
  type(C_FUNPTR), public :: getcuriter
  type(C_FUNPTR), public :: getnumconvfails
 end type SUNNonlinearSolver_Ops
```

10.1.7 Usage with sensitivity enabled integrators

When used with SUNDIALS packages that support sensitivity analysis capabilities (e.g., CVODES and IDAS) a special NVECTOR module is used to interface with SUNNONLINSOL modules for solves involving

sensitivity vectors stored in an NVECTOR array. As described below, the NVECTOR_SENSWRAPPER module is an NVECTOR implementation where the vector content is an NVECTOR array. This wrapper vector allows SUNNONLINSOL modules to operate on data stored as a collection of vectors.

For all SUNDIALS-provided SUNNONLINSOL modules a special constructor wrapper is provided so users do not need to interact directly with the NVECTOR_SENSWRAPPER module. These constructors follow the naming convention `SUNNonlinSol_***Sens(count,...)` where `***` is the name of the SUNNONLINSOL module, `count` is the size of the vector wrapper, and `...` are the module-specific constructor arguments.

The NVECTOR_SENSWRAPPER module

This section describes the NVECTOR_SENSWRAPPER implementation of an NVECTOR. To access the NVECTOR_SENSWRAPPER module, include the header file
`sundials/sundials_nvector_senswrapper.h`.

The NVECTOR_SENSWRAPPER module defines an `N_Vector` implementing all of the standard vectors operations defined in Table 7.1.1 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`.

F2003 Name `FN_VNewEmpty_SensWrapper`

`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`.

F2003 Name `FN_VNew_SensWrapper`

The NVECTOR_SENSWRAPPER implementation of the NVECTOR module defines the *content* field of the `N_Vector` to be a structure containing an `N_Vector` array, the number of vectors in the vector array, and a boolean flag indicating ownership of the vectors in the vector array.

```
struct _N_VectorContent_SensWrapper {
  N_Vector* vecs;
  int nvecs;
  booleantype own_vecs;
};
```

The following macros are provided to access the content of an NVECTOR_SENSWRAPPER vector.

- `NV_CONTENT_SW(v)` - provides access to the content structure
- `NV_VECS_SW(v)` - provides access to the vector array
- `NV_NVECS_SW(v)` - provides access to the number of vectors
- `NV_OWN_VECS_SW(v)` - provides access to the ownership flag
- `NV_VEC_SW(v,i)` - provides access to the `i`-th vector in the vector array

10.1.8 Implementing a Custom SUNNonlinearSolver Module

A SUNNONLINSOL implementation *must* do the following:

1. Specify the content of the SUNNONLINSOL module.
2. Define and implement the required nonlinear solver operations defined in Sections 10.1.1 – 10.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one SUNNONLINSOL module (each with different `SUNNonlinearSolver` internal data representations) in the same code.
3. Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

1. Define and implement additional user-callable "set" routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.
2. Provide additional user-callable "get" routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

To aid in the creation of custom SUNNONLINSOL modules the generic SUNNONLINSOL module provides the utility functions `SUNNonlinSolNewEmpty` and `SUNNonlinsolFreeEmpty`. When used in custom SUNNONLINSOL constructors, the function `SUNNonlinSolNewEmpty` will ease the introduction of any new optional nonlinear solver operations to the SUNNONLINSOL API by ensuring only required operations need to be set.

`SUNNonlinSolNewEmpty`

Call `NLS = SUNNonlinSolNewEmpty();`

Description The function `SUNNonlinSolNewEmpty` allocates a new generic SUNNONLINSOL object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

Arguments None

Return value This function returns a `SUNNonlinearSolver` object. If an error occurs when allocating the object, then this routine will return `NULL`.

F2003 Name `FSUNNonlinSolNewEmpty`

`SUNNonlinSolFreeEmpty`

Call `SUNNonlinSolFreeEmpty(NLS);`

Description This routine frees the generic `SUNNonlinearSolver` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `NLS` (`SUNNonlinearSolver`)

Return value None

F2003 Name `FSUNNonlinSolFreeEmpty`

10.2 IDA SUNNonlinearSolver interface

As discussed in Chapter 2 each integration step requires the (approximate) solution of the nonlinear system

$$G(y_n) = F\left(t_n, y_n, h_n^{-1}\sum_{i=0}^{q}\alpha_{n,i}y_{n-i}\right) = 0. \tag{10.1}$$

Rather than solving this system for the new state y_n IDA reformulates the system to solve for the correction y_{cor} to the predicted new state y_{pred} and its derivative $\dot{y}_{pred}$ so that $y_n = y_{pred} + y_{cor}$ and $\dot{y}_n = \dot{y}_{pred} + h_n^{-1}\alpha_{n,0}y_{cor}$. The nonlinear system rewritten in terms of y_{cor} is

$$G(y_{cor}) = F\left(t_n, y_{pred} + y_{cor}, \dot{y}_{pred} + \alpha y_{cor}\right) = 0. \tag{10.2}$$

where $\alpha = h_n^{-1}\alpha_{n,0}$.

The nonlinear system function provided by IDA to the nonlinear solver module internally updates the current value of the new state and its derivative based on the input correction vector. The updated vectors are used when calling the DAE residual function and when setting up linear solves (e.g., for updating the Jacobian or preconditioner).

IDA provides several advanced functions that will not be needed by most users, but might be useful for users who choose to provide their own implementation of the `SUNNonlinearSolver` API. For example, such a user might need access to the current y and $\dot{y}$ vectors to compute Jacobian data.

`IDAGetCurrentCj`

Call `flag = IDAGetCurrentCj(ida_mem, &cj);`

Description The function `IDAGetCurrentCj` returns the scalar c_j which is proportional to the inverse of the step size (α in (10.2)).

Arguments `ida_mem` (`void *`) pointer to the IDA memory block.
`cj` (`realtype`) the value of c_j.

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`.

F2003 Name `FIDAGetCurrentCj`

`IDAGetCurrentY`

Call `flag = IDAGetCurrentY(ida_mem, &y);`

Description The function `IDAGetCurrentY` returns the current y vector.

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

`y` (`N_Vector *`) the current y vector

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

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

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

F2003 Name `FIDAGetCurrentY`

`IDAGetCurrentYp`

Call `flag = IDAGetCurrentYp(ida_mem, &yp);`

Description The function `IDAGetCurrentYp` returns the current $\dot{y}$ vector.

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

`yp` (`N_Vector *`) the current $\dot{y}$ vector

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

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

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

F2003 Name `FIDAGetCurrentYp`

`IDAGetNonlinearSystemData`

Call `flag = IDAGetNonlinearSystemData(ida_mem, &tcur, &yypred, &yppred, &yyn, &ypn, &res, &cj, user_data);`

Description The function `IDAGetNonlinearSystemData` returns all internal data required to construct the current nonlinear system (10.2).

Arguments

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

`tcur` (`realtype*`) current value of the independent variable t_n.

`yypred` (`N_Vector*`) predicted value of y_{pred} at t_n.

`yppred` (`N_Vector*`) predicted value of $\dot{y}_{pred}$ at t_n.

`yyn` (`N_Vector*`) the vector y_n. This vector may be not current and may need to be filled (see the note below).

`ypn` (`N_Vector*`) the vector $\dot{y}_n$. This vector may be not current and may need to be filled (see the note below).

`res` (`N_Vector*`) the resiudal function evaluated at the current time and state, $F(t_n, y_n, \dot{y}_n)$. This vector may be not current and may need to be filled (see the note below).

`cj` (`realtype*`) the scalar c_j which is proportional to the inverse of the step size (α in (10.2)).

`user_data` (`void**`) pointer to the user-defined data structures

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 This routine is intended for users who wish to attach a custom `SUNNonlinSolSysFn` (see §10.1.4) to an existing `SUNNonlinearSolver` object (through a call to `SUNNonlinSolSetSysFn`) or who need access to nonlinear system data to compute the nonlinear system fucntion as part of a custom `SUNNonlinearSolver` object.

When supplying a custom `SUNNonlinSolSysFn` to an existing `SUNNonlinearSolver` object, the user should call `IDAGetNonlinearSystemData` **inside** the nonlinear system function to access the requisite data for evaluting the nonlinear system function of their choosing. Additionlly, if the `SUNNonlinearSolver` object (existing or custom) leverages the `SUNNonlinSolLSetupFn` and/or `SUNNonlinSolLSolveFn` functions supplied by IDA (through calls to `SUNNonlinSolSetLSetupFn` and `SUNNonlinSolSetLSolveFn` respectively) the vectors `yyn`, `ypn`, and `res` **must be filled** in by the user's `SUNNonlinSolSysFn` with the current state and corresponding evaluation of the right-hand side function respectively i.e.,

$$\begin{aligned} yyn &= y_{pred} + y_{cor}, \\ ypn &= \dot{y}_{pred} + \alpha \dot{y}_{cor}, \\ res &= F\left(t_n, y_n, \dot{y}_n\right), \end{aligned}$$

where y_{cor} was the first argument supplied to the `SUNNonlinSolSysFn`.

If this function is called as part of a custom linear solver (i.e., the default `SUNNonlinSolSysFn` is used) then the vectors `yyn`, `ypn`, and `res` are only current when `IDAGetNonlinearSystemData` is called after an evaluation of the nonlinear system function.

F2003 Name `FIDAGetNonlinearSystemData`

`IDAComputeY`

Call `flag = IDAComputeY(ida_mem, ycor, y);`

Description The function computes the current $y(t)$ vector based on the given correction vector from the nonlinear solver.

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

`ycor` (`N_Vector`) the correction

`y` (`N_Vector`) the output vector

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

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

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

F2003 Name `FIDAComputeY`

`IDAComputeYp`

Call `flag = IDAComputeYp(ida_mem, ycor, yp);`

Description The function computes $\dot{y}(t)$.

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

`ycor` (`N_Vector`) the correction

`yp` (`N_Vector`) the output vector array

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.

F2003 Name FIDAComputeYp

10.3 The SUNNonlinearSolver_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton's method. To access the SUNNONLINSOL_NEWTON module, include the header file sunnonlinsol/sunnonlinsol_newton.h. We note that the SUNNONLINSOL_NEWTON module is accessible from SUNDIALS integrators *without* separately linking to the libsundials_sunnonlinsolnewton module library.

10.3.1 SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{10.3}$$

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

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{10.4}$$

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

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)}), \tag{10.5}$$

in which A is the Jacobian matrix

$$A \equiv \partial F/\partial y\,. \tag{10.6}$$

Depending on the linear solver used, the SUNNONLINSOL_NEWTON module will employ either a Modified Newton method, or an Inexact Newton method [12, 16, 23, 25, 38]. When used with a direct linear solver, the Jacobian matrix A is held constant during the Newton iteration, resulting in a Modified Newton method. With a matrix-free iterative linear solver, the iteration is an Inexact Newton method.

In both cases, calls to the integrator-supplied SUNNonlinSolLSetupFn function are made infrequently to amortize the increased cost of matrix operations (updating A and its factorization within direct linear solvers, or updating the preconditioner within iterative linear solvers). Specifically, SUNNONLINSOL_NEWTON will call the SUNNonlinSolLSetupFn function in two instances:

(a) when requested by the integrator (the input callLSetSetup is SUNTRUE) before attempting the Newton iteration, or

(b) when reattempting the nonlinear solve after a recoverable failure occurs in the Newton iteration with stale Jacobian information (jcur is SUNFALSE). In this case, SUNNONLINSOL_NEWTON will set jbad to SUNTRUE before calling the SUNNonlinSolLSetupFn function.

Whether the Jacobian matrix A is fully or partially updated depends on logic unique to each integrator-supplied SUNNonlinSolSetupFn routine. We refer to the discussion of nonlinear solver strategies provided in Chapter 2 for details on this decision.

The default maximum number of iterations and the stopping criteria for the Newton iteration are supplied by the SUNDIALS integrator when SUNNONLINSOL_NEWTON is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling the SUNNonlinSolSetMaxIters and/or SUNNonlinSolSetConvTestFn functions after attaching the SUNNONLINSOL_NEWTON object to the integrator.

10.3.2 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 `FSUNNonlinSol_Newton`

`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 `FSUNNonlinSol_NewtonSens`

The SUNNONLINSOL_NEWTON module implements all of the functions defined in sections 10.1.1 – 10.1.3 except for the `SUNNonlinSolSetup` function. The SUNNONLINSOL_NEWTON functions have the same names as those defined by the generic SUNNONLINSOL API with `_Newton` appended to the function name. Unless using the SUNNONLINSOL_NEWTON module as a standalone nonlinear solver the generic functions defined in sections 10.1.1 – 10.1.3 should be called in favor of the SUNNONLINSOL_NEWTON-specific implementations.

The SUNNONLINSOL_NEWTON module also defines the following additional user-callable function.

`SUNNonlinSolGetSysFn_Newton`

Call `retval = SUNNonlinSolGetSysFn_Newton(NLS, SysFn);`

Description The function `SUNNonlinSolGetSysFn_Newton` returns the residual function that defines the nonlinear system.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object

`SysFn` (`SUNNonlinSolSysFn*`) the function defining the nonlinear system.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes This function is intended for users that wish to evaluate the nonlinear residual in a custom convergence test function for the SUNNONLINSOL_NEWTON module. We note that SUNNONLINSOL_NEWTON will not leverage the results from any user calls to `SysFn`.

F2003 Name `FSUNNonlinSolGetSysFn_Newton`

`SUNNonlinSolSetInfoFile_Newton`

Call `retval = SUNNonlinSolSetInfoFile_Newton(NLS, info_file);`

Description The function `SUNNonlinSolSetInfoFile_Newton` sets the output file where all informative (non-error) messages should be directed.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
- `info_file` (`FILE*`) pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value The return value is

- `SUN_NLS_SUCCESS` if successful
- `SUN_NLS_MEM_NULL` if the SUNNonlinearSolver memory was `NULL`
- `SUN_NLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled

Notes This function is intended for users that wish to monitor the nonlinear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNNonlinSolSetInfoFile_Newton`

`SUNNonlinSolSetPrintLevel_Newton`

Call `retval = SUNNonlinSolSetPrintLevel_Newton(NLS, print_level);`

Description The function `SUNNonlinSolSetPrintLevel_Newton` specifies the level of verbosity of the output.

Arguments
- `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
- `print_level` (`int`) flag indicating level of verbosity; must be one of:
  - 0, no information is printed (default)
  - 1, for each nonlinear iteration the residual norm is printed

Return value The return value is

- `SUN_NLS_SUCCESS` if successful
- `SUN_NLS_MEM_NULL` if the SUNNonlinearSolver memory was `NULL`
- `SUN_NLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid

Notes This function is intended for users that wish to monitor the nonlinear solver progress. By default, the print level is 0.

SUNDIALS **must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING`, to utilize this function.** See section A.1.2 for more information.

F2003 Name `FSUNNonlinSolSetPrintLevel_Newton`

10.3.3 SUNNonlinearSolver_Newton Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

For SUNDIALS integrators that include a FORTRAN 77 interface, the SUNNONLINSOL_NEWTON module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

`FSUNNEWTONINIT`

Call `FSUNNEWTONINIT(code, ier);`

Description The function `FSUNNEWTONINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ with Newton's method.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

10.3.4 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;
  void*       ctest_data;

  int print_level;
  FILE* info_file;
};
```

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,
`niters` - the total number of nonlinear iterations across all solves,
`nconvfails` - the total number of nonlinear convergence failures across all solves, and
`ctest_data` - the data pointer passed to the convergence test function.
`print_level` - controls the amount of information to be printed to the info file
`info_file` - the file where all informative (non-error) messages will be directed

10.4 The SUNNonlinearSolver_PetscSNES implementation

This section describes the SUNNONLINSOL interface to the PETSc SNES nonlinear solver(s). To enable the SUNNONLINSOL_PETSCSNES module, SUNDIALS must be configured to use PETSc. Instructions on how to do this are given in Chapter A.1.4. To access the module, users must include the header file `sunnonlinsol/sunnonlinsol_petscsnes.h`. The library to link to is `libsundials_sunnonlinsolpetsc`.*lib* where *.lib* is .so for shared libaries and .a for static libraries. Users of the SUNNONLINSOL_PETSCSNES should also see the section NVECTOR_PETSC 7.8 which discusses the NVECTOR interface to the PETSc Vec API.

10.4.1 SUNNonlinearSolver_PetscSNES description

The SUNNONLINSOL_PETSCSNES implementation allows users to utilize a PETSc SNES nonlinear solver to solve the nonlinear systems that arise in the SUNDIALS integrators. Since SNES uses the KSP linear solver interface underneath it, the SUNNONLINSOL_PETSCSNES implementation does not interface with SUNDIALS linear solvers. Instead, users should set nonlinear solver options, linear solver options, and preconditioner options through the PETSc SNES, KSP, and PC APIs [10].

Important usage notes for the SUNNONLINSOL_PETSCSNES implementation are provided below:

- The SUNNONLINSOL_PETSCSNES implementation handles calling `SNESSetFunction` at construction. The actual residual function $F(y)$ is set by the SUNDIALS integrator when the SUNNONLINSOL_PETSCSNES object is attached to it. Therefore, a user should not call `SNESSetFunction` on a `SNES` object that is being used with SUNNONLINSOL_PETSCSNES. For these reasons, it is recommended, although not always necessary, that the user calls `SUNNonlinSol_PetscSNES` with the new `SNES` object immediately after calling
- The number of nonlinear iterations is tracked by SUNDIALS separately from the count kept by SNES. As such, the function `SUNNonlinSolGetNumIters` reports the cumulative number of iterations across the lifetime of the SUNNONLINSOL object.
- Some "converged" and "diverged" convergence reasons returned by SNES are treated as recoverable convergence failures by SUNDIALS. Therefore, the count of convergence failures returned by `SUNNonlinSolGetNumConvFails` will reflect the number of recoverable convergence failures as determined by SUNDIALS, and may differ from the count returned by `SNESGetNonlinearStepFailures`.
- The SUNNONLINSOL_PETSCSNES module is not currently compatible with the CVODES or IDAS staggered or simultaneous sensitivity strategies.

10.4.2 SUNNonlinearSolver_PetscSNES functions

The SUNNONLINSOL_PETSCSNES module provides the following constructor for creating a `SUNNonlinearSolver` object.

`SUNNonlinSol_PetscSNES`

Call `NLS = SUNNonlinSol_PetscSNES(y, snes);`

Description The function `SUNNonlinSol_PetscSNES` creates a `SUNNonlinearSolver` object that wraps a PETSc `SNES` object for use with SUNDIALS. This will call `SNESSetFunction` on the provided `SNES` object.

Arguments `snes` (`SNES`) a PETSc `SNES` object

`y` (`N_Vector`) a `N_Vector` object of type NVECTOR_PETSC that used as a template for the residual vector

Return value A SUNNONLINSOL object if the constructor exits successfully, otherwise `NLS` will be `NULL`.

Notes This function calls `SNESSetFunction` and will overwrite whatever function was previously set. Users should not call `SNESSetFunction` on the `SNES` object provided to the constructor.

The SUNNONLINSOL_PETSCSNES module implements all of the functions defined in sections 10.1.1 – 10.1.3 except for `SUNNonlinSolSetup`, `SUNNonlinSolSetLSetupFn`, `SUNNonlinSolSetLSolveFn`, `SUNNonlinSolSetConvTestFn`, and `SUNNonlinSolSetMaxIters`.

The SUNNONLINSOL_PETSCSNES functions have the same names as those defined by the generic SUNNONLINSOL API with `_PetscSNES` appended to the function name. Unless using the SUNNONLINSOL_PETSCSNES module as a standalone nonlinear solver the generic functions defined in sections 10.1.1 – 10.1.3 should be called in favor of the SUNNONLINSOL_PETSCSNES-specific implementations.

The SUNNONLINSOL_PETSCSNES module also defines the following additional user-callable functions.

`SUNNonlinSolGetSNES_PetscSNES`

Call `retval = SUNNonlinSolGetSNES_PetscSNES(NLS, SNES* snes);`

Description The function `SUNNonlinSolGetSNES_PetscSNES` gets the SNES context that was wrapped.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object

`snes` (`SNES*`) a pointer to a PETSc `SNES` object that will be set upon return

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

`SUNNonlinSolGetPetscError_PetscSNES`

Call `retval = SUNNonlinSolGetPetscError_PetscSNES(NLS, PestcErrorCode* error);`

Description The function `SUNNonlinSolGetPetscError_PetscSNES` gets the last error code returned by the last internal call to a PETSc API function.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object

`error` (`PestcErrorCode*`) a pointer to a PETSc error integer that will be set upon return

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

`SUNNonlinSolGetSysFn_PetscSNES`

Call `retval = SUNNonlinSolGetSysFn_PetscSNES(NLS, SysFn);`

Description The function `SUNNonlinSolGetSysFn_PetscSNES` 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.

10.4.3 SUNNonlinearSolver_PetscSNES content

The SUNNONLINSOL_PETSCSNES module defines the *content* field of a `SUNNonlinearSolver` as the following structure:

```
struct _SUNNonlinearSolverContent_PetscSNES {
  int sysfn_last_err;
  PetscErrorCode petsc_last_err;
  long int nconvfails;
  long int nni;
  void *imem;
  SNES snes;
  Vec r;
  N_Vector y, f;
  SUNNonlinSolSysFn Sys;
};
```

These entries of the *content* field contain the following information:
`sysfn_last_err` - last error returned by the system defining function,

`petsc_last_err` - last error returned by PETSc

`nconvfails` - number of nonlinear converge failures (recoverable or not),

`nni` - number of nonlinear iterations,

`imem` - SUNDIALS integrator memory,

`snes` - PETSc SNES context,

`r` - the nonlinear residual,

`y` - wrapper for PETSc vectors used in the system function,

`f` - wrapper for PETSc vectors used in the system function,

`Sys` - nonlinear system definining function.

Chapter 11

Description of the SUNMemory module

To support applications which leverage memory pools, or utilize a memory abstraction layer, SUNDIALS provides a set of utilities we will collectively refer to as the `SUNMemoryHelper` API. The goal of this API is to allow users to leverage operations defined by native SUNDIALS data structures while allowing the user to have finer-grained control of the memory management.

11.1 The SUNMemoryHelper API

This API consists of three new SUNDIALS types: `SUNMemoryType`, `SUNMemory`, and `SUNMemoryHelper`, which we now define.

The `SUNMemory` structure wraps a pointer to actual data. This structure is defined as

```
typedef struct _SUNMemory
{
  void*         ptr;
  SUNMemoryType type;
  booleantype   own;
} *SUNMemory;
```

The `SUNMemoryType` type is an enumeration that defines the four supported memory types:

```
typedef enum
{
  SUNMEMTYPE_HOST,      /* pageable memory accessible on the host     */
  SUNMEMTYPE_PINNED,    /* page-locked memory accesible on the host   */
  SUNMEMTYPE_DEVICE,    /* memory accessible from the device          */
  SUNMEMTYPE_UVM        /* memory accessible from the host or device  */
} SUNMemoryType;
```

Finally, the `SUNMemoryHelper` structure is defined as

```
struct _SUNMemoryHelper
{
  void*               content;
  SUNMemoryHelper_Ops ops;
} *SUNMemoryHelper;
```

where `SUNMemoryHelper_Ops` is defined as

```
typedef struct _SUNMemoryHelper_Ops
{
  /* operations that implementations are required to provide */
  int             (*alloc)(SUNMemoryHelper, SUNMemory* memptr, size_t mem_size, SUNMemoryType mem_typ
  int             (*dealloc)(SUNMemoryHelper, SUNMemory mem);
  int             (*copy)(SUNMemoryHelper, SUNMemory dst, SUNMemory src, size_t mem_size);

  /* operations that provide default implementations */
  int             (*copyasync)(SUNMemoryHelper, SUNMemory dst, SUNMemory src,
                               size_t mem_size, void* ctx);
  SUNMemoryHelper (*clone)(SUNMemoryHelper);
  int             (*destroy)(SUNMemoryHelper);
} *SUNMemoryHelper_Ops;
```

11.1.1 Implementation defined operations

The SUNMemory API also defines the following operations which do require a SUNMemoryHelper instance and **require** the implementation to define them:

`SUNMemoryHelper_Alloc`

Call `retval = SUNMemoryHelper_Alloc(helper, *memptr, mem_size, mem_type);`

Description Allocates a SUNMemory object whose ptr field is allocated for mem_size bytes and is of type mem_type. The new object will have ownership of ptr and will be deallocated when SUNMemoryHelper_Dealloc is called.

Arguments
- `helper` (SUNMemoryHelper) the SUNMemoryHelper object
- `memptr` (SUNMemory*) pointer to the allocated SUNMemory
- `mem_size` (size_t) the size in bytes of the ptr
- `mem_type` (SUNMemoryType) the SUNMemoryType of the ptr

Return value An int flag indicating success (zero) or failure (non-zero).

`SUNMemoryHelper_Dealloc`

Call `retval = SUNMemoryHelper_Dealloc(helper, mem);`

Description Deallocates the mem->ptr field if it is owned by mem, and then deallocates the mem object.

Arguments
- `helper` (SUNMemoryHelper) the SUNMemoryHelper object
- `mem` (SUNMemory) the SUNMemory object

Return value An int flag indicating success (zero) or failure (non-zero).

`SUNMemoryHelper_Copy`

Call `retval = SUNMemoryHelper_Copy(helper, dst, src, mem_size);`

Description Synchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object should use the memory types of dst and src to determine the appropriate transfer type necessary.

Arguments
- `helper` (SUNMemoryHelper) the SUNMemoryHelper object
- `dst` (SUNMemory) the destination memory to copy to
- `src` (SUNMemory) the source memory to copy from
- `mem_size` (size_t) the number of bytes to copy

Return value An int flag indicating success (zero) or failure (non-zero).

11.1.2 Utility Functions

The SUNMemoryHelper API defines the following functions which do not require a SUNMemoryHelper instance:

SUNMemoryHelper_Alias

Call `mem2 = SUNMemoryHelper_Alias(mem1);`

Description Returns a SUNMemory object whose ptr field points to the same address as mem1. The new object *will not* have ownership of ptr, therefore, it will not free ptr when SUNMemoryHelper_Dealloc is called.

Arguments `mem1` (SUNMemory) a SUNMemory object

Return value A SUNMemory object.

SUNMemoryHelper_Wrap

Call `mem = SUNMemoryHelper_Wrap(ptr, mem_type);`

Description Returns a SUNMemory object whose ptr field points to the ptr argument passed to the function. The new object *will not* have ownership of ptr, therefore, it will not free ptr when SUNMemoryHelper_Dealloc is called.

Arguments `ptr` (SUNMemoryType) the data pointer to wrap in a SUNMemory object
`mem_type` (SUNMemoryType) the SUNMemoryType of the ptr

Return value A SUNMemory object.

SUNMemoryHelper_NewEmpty

Call `helper = SUNMemoryHelper_NewEmpty();`

Description Returns an empty SUNMemoryHelper. This is useful for building custom SUNMemoryHelper implementations.

Arguments

Return value A SUNMemoryHelper object.

SUNMemoryHelper_CopyOps

Call `retval = SUNMemoryHelper_CopyOps(src, dst);`

Description Copies the ops field of src to the ops field of dst. This is useful for building custom SUNMemoryHelper implementations.

Arguments `src` (SUNMemoryHelper) the object to copy from
`dst` (SUNMemoryHelper) the object to copy to

Return value An int flag indicating success (zero) or failure (non-zero).

11.1.3 Implementation overridable operations with defaults

In addition, the SUNMemoryHelper API defines the following *optionally overridable* operations which do require a SUNMemoryHelper instance:

`SUNMemoryHelper_CopyAsync`

Call `retval = SUNMemoryHelper_CopyAsync(helper, dst, src, mem_size, ctx);`

Description Asynchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object should use the memory types of `dst` and `src` to determine the appropriate transfer type necessary. The `ctx` argument is used when a different execution "stream" needs to be provided to perform the copy in, e.g. with `CUDA` this would be a `cudaStream_t`.

Arguments
- `helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object
- `dst` (`SUNMemory`) the destination memory to copy to
- `src` (`SUNMemory`) the source memory to copy from
- `mem_size` (`size_t`) the number of bytes to copy
- `ctx` (`void *`) typically a handle for an object representing an alternate execution stream, but it can be any implementation specific data

Return value An `int` flag indicating success (zero) or failure (non-zero).

Notes If this operation is not defined by the implementation, then `SUNMemoryHelper_Copy` will be used.

`SUNMemoryHelper_Clone`

Call `helper2 = SUNMemoryHelper_Clone(helper);`

Description Clones the `SUNMemoryHelper` object itself.

Arguments `helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object to clone

Return value A `SUNMemoryHelper` object.

Notes If this operation is not defined by the implementation, then the default clone will only copy the `SUNMemoryHelper_Ops` structure stored in `helper->ops`, and not the `helper->content` field.

`SUNMemoryHelper_Destroy`

Call `retval = SUNMemoryHelper_Destroy(helper);`

Description Destroys (frees) the `SUNMemoryHelper` object itself.

Arguments `helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object to destroy

Return value An `int` flag indicating success (zero) or failure (non-zero).

Notes If this operation is not defined by the implementation, then the default destroy will only free the `helper->ops` field and the `helper` itself. The `helper->content` field will not be freed.

11.1.4 Implementing a custom `SUNMemoryHelper`

A particular implementation of the `SUNMemoryHelper` API must:

- Define and implement the required operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one `SUNMemoryHelper` module in the same code.
- Optionally, specify the *content* field of `SUNMemoryHelper`.
- Optionally, define and implement additional user-callable routines acting on the newly defined `SUNMemoryHelper`.

An example of a custom `SUNMemoryHelper` is given in `examples/utilities/custom_memory_helper.h`.

11.2 The SUNMemoryHelper_Cuda implementation

The SUNMemoryHelper_Cuda module is an implementation of the SUNMemoryHelper API that interfaces to the NVIDIA CUDA [5] library. The implementation defines the constructor

SUNMemoryHelper_Cuda	
Call	`helper = SUNMemoryHelper_Cuda();`
Description	Allocates and returns a SUNMemoryHelper object for handling CUDA memory.
Arguments	None
Return value	A SUNMemoryHelper object if successful, or NULL if not.

11.2.1 SUNMemoryHelper API functions

The implementation provides the following operations defined by the SUNMemoryHelper API:

SUNMemoryHelper_Alloc_Cuda	
Call	`retval = SUNMemoryHelper_Alloc_Cuda(helper, *memptr, mem_size, mem_type);`
Description	Allocates a SUNMemory object whose ptr field is allocated for mem_size bytes and is of type mem_type. The new object will have ownership of ptr and will be deallocated when SUNMemoryHelper_Dealloc is called. The SUNMemoryType supported are • SUNMEMTYPE_HOST – memory is allocated with a call to malloc • SUNMEMTYPE_PINNED – memory is allocated with a call to cudaMallocHost • SUNMEMTYPE_DEVICE – memory is allocated with a call to cudaMalloc • SUNMEMTYPE_UVM – memory is allocated with a call to cudaMallocManaged
Arguments	helper (SUNMemoryHelper) the SUNMemoryHelper object memptr (SUNMemory*) pointer to the allocated SUNMemory mem_size (size_t) the size in bytes of the ptr mem_type (SUNMemoryType) the SUNMemoryType of the ptr
Return value	An int flag indicating success (zero) or failure (non-zero).

SUNMemoryHelper_Dealloc_Cuda	
Call	`retval = SUNMemoryHelper_Dealloc_Cuda(helper, mem);`
Description	Deallocates the mem->ptr field if it is owned by mem, and then deallocates the mem object.
Arguments	helper (SUNMemoryHelper) the SUNMemoryHelper object mem (SUNMemory) the SUNMemory object
Return value	An int flag indicating success (zero) or failure (non-zero).

SUNMemoryHelper_Copy_Cuda	
Call	`retval = SUNMemoryHelper_Copy_Cuda(helper, dst, src, mem_size);`
Description	Synchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object will use the memory types of dst and src to determine the appropriate transfer type necessary.
Arguments	This operation uses cudaMemcpy underneath.

Return value	`helper`	(`SUNMemoryHelper`) the `SUNMemoryHelper` object
	`dst`	(`SUNMemory`) the destination memory to copy to
	`src`	(`SUNMemory`) the source memory to copy from
	`mem_size`	(`size_t`) the number of bytes to copy
Notes	An `int` flag indicating success (zero) or failure (non-zero).	

`SUNMemoryHelper_CopyAsync_Cuda`

Call `retval = SUNMemoryHelper_CopyAsync_Cuda(helper, dst, src, mem_size, ctx);`

Description Asynchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments This operation uses `cudaMemcpyAsync` underneath.

Return value	`helper`	(`SUNMemoryHelper`) the `SUNMemoryHelper` object
	`dst`	(`SUNMemory`) the destination memory to copy to
	`src`	(`SUNMemory`) the source memory to copy from
	`mem_size`	(`size_t`) the number of bytes to copy
	`ctx`	(`void *`) the `cudaStream_t` handle for the stream that the copy will be performed on
Notes	An `int` flag indicating success (zero) or failure (non-zero).	

11.3 The `SUNMemoryHelper_Hip` implementation

The `SUNMemoryHelper_Hip` module is an implementation of the `SUNMemoryHelper` API that interfaces to the AMD ROCm HIP library. The implementation defines the constructor

`SUNMemoryHelper_Hip`

Call `helper = SUNMemoryHelper_Hip();`

Description Allocates and returns a `SUNMemoryHelper` object for handling HIP memory.

Arguments None

Return value A `SUNMemoryHelper` object if successful, or `NULL` if not.

11.3.1 `SUNMemoryHelper` API functions

The implementation provides the following operations defined by the `SUNMemoryHelper` API:

`SUNMemoryHelper_Alloc_Hip`

Call `retval = SUNMemoryHelper_Alloc_Hip(helper, *memptr, mem_size, mem_type);`

Description Allocates a `SUNMemory` object whose `ptr` field is allocated for `mem_size` bytes and is of type `mem_type`. The new object will have ownership of `ptr` and will be deallocated when `SUNMemoryHelper_Dealloc` is called.

The `SUNMemoryType` supported are

- `SUNMEMTYPE_HOST` – memory is allocated with a call to `malloc`
- `SUNMEMTYPE_PINNED` – memory is allocated with a call to `hipMallocHost`
- `SUNMEMTYPE_DEVICE` – memory is allocated with a call to `hipMalloc`

- SUNMEMTYPE_UVM – memory is allocated with a call to hipMallocManaged

Arguments
- helper (SUNMemoryHelper) the SUNMemoryHelper object
- memptr (SUNMemory*) pointer to the allocated SUNMemory
- mem_size (size_t) the size in bytes of the ptr
- mem_type (SUNMemoryType) the SUNMemoryType of the ptr

Return value An int flag indicating success (zero) or failure (non-zero).

SUNMemoryHelper_Dealloc_Hip

Call `retval = SUNMemoryHelper_Dealloc_Hip(helper, mem);`

Description Deallocates the mem->ptr field if it is owned by mem, and then deallocates the mem object.

Arguments
- helper (SUNMemoryHelper) the SUNMemoryHelper object
- mem (SUNMemory) the SUNMemory object

Return value An int flag indicating success (zero) or failure (non-zero).

SUNMemoryHelper_Copy_Hip

Call `retval = SUNMemoryHelper_Copy_Hip(helper, dst, src, mem_size);`

Description Synchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object will use the memory types of dst and src to determine the appropriate transfer type necessary.

Arguments This operation uses hipMemcpy underneath.

Return value
- helper (SUNMemoryHelper) the SUNMemoryHelper object
- dst (SUNMemory) the destination memory to copy to
- src (SUNMemory) the source memory to copy from
- mem_size (size_t) the number of bytes to copy

Notes An int flag indicating success (zero) or failure (non-zero).

SUNMemoryHelper_CopyAsync_Hip

Call `retval = SUNMemoryHelper_CopyAsync_Hip(helper, dst, src, mem_size, ctx);`

Description Asynchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object will use the memory types of dst and src to determine the appropriate transfer type necessary.

Arguments This operation uses hipMemcpyAsync underneath.

Return value
- helper (SUNMemoryHelper) the SUNMemoryHelper object
- dst (SUNMemory) the destination memory to copy to
- src (SUNMemory) the source memory to copy from
- mem_size (size_t) the number of bytes to copy
- ctx (void *) the hipStream_t handle for the stream that the copy will be performed on

Notes An int flag indicating success (zero) or failure (non-zero).

11.4 The SUNMemoryHelper_Sycl implementation

The SUNMemoryHelper_Sycl module is an implementation of the SUNMemoryHelper API that interfaces to the SYCL abstraction layer. The implementation defines the constructor

`SUNMemoryHelper_Sycl`

Call `helper = SUNMemoryHelper_Sycl(Q);`

Description Allocates and returns a `SUNMemoryHelper` object for handling SYCL memory.

Arguments `Q` (`sycl::queue`) the queue to use for memory operations

Return value A `SUNMemoryHelper` object if successful, or `NULL` if not.

11.4.1 `SUNMemoryHelper` API functions

The implementation provides the following operations defined by the `SUNMemoryHelper` API:

`SUNMemoryHelper_Alloc_Sycl`

Call `retval = SUNMemoryHelper_Alloc_Sycl(helper, *memptr, mem_size, mem_type);`

Description Allocates a `SUNMemory` object whose `ptr` field is allocated for `mem_size` bytes and is of type `mem_type`. The new object will have ownership of `ptr` and will be deallocated when `SUNMemoryHelper_Dealloc` is called.

The `SUNMemoryType` supported are

- `SUNMEMTYPE_HOST` – memory is allocated with a call to `malloc`
- `SUNMEMTYPE_PINNED` – memory is allocated with a call to `sycl::malloc_host`
- `SUNMEMTYPE_DEVICE` – memory is allocated with a call to `sycl::malloc_device`
- `SUNMEMTYPE_UVM` – memory is allocated with a call to `sycl::malloc_shared`

Arguments
`helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object
`memptr` (`SUNMemory*`) pointer to the allocated `SUNMemory`
`mem_size` (`size_t`) the size in bytes of the `ptr`
`mem_type` (`SUNMemoryType`) the `SUNMemoryType` of the `ptr`

Return value An `int` flag indicating success (zero) or failure (non-zero).

`SUNMemoryHelper_Dealloc_Sycl`

Call `retval = SUNMemoryHelper_Dealloc_Sycl(helper, mem);`

Description Deallocates the `mem->ptr` field if it is owned by `mem`, and then deallocates the `mem` object.

Arguments
`helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object
`mem` (`SUNMemory`) the `SUNMemory` object

Return value An `int` flag indicating success (zero) or failure (non-zero).

`SUNMemoryHelper_Copy_Sycl`

Call `retval = SUNMemoryHelper_Copy_Sycl(helper, dst, src, mem_size);`

Description Synchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments This operation uses `syclMemcpy` underneath.

Return value
`helper` (`SUNMemoryHelper`) the `SUNMemoryHelper` object
`dst` (`SUNMemory`) the destination memory to copy to
`src` (`SUNMemory`) the source memory to copy from
`mem_size` (`size_t`) the number of bytes to copy

Notes An `int` flag indicating success (zero) or failure (non-zero).

`SUNMemoryHelper_CopyAsync_Sycl`

Call `retval = SUNMemoryHelper_CopyAsync_Sycl(helper, dst, src, mem_size, ctx);`

Description Asynchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments This operation uses `syclMemcpyAsync` underneath.

Return value

`helper`	(`SUNMemoryHelper`) the `SUNMemoryHelper` object
`dst`	(`SUNMemory`) the destination memory to copy to
`src`	(`SUNMemory`) the source memory to copy from
`mem_size`	(`size_t`) the number of bytes to copy
`ctx`	(`void *`) is unsued in this function

Notes An `int` flag indicating success (zero) or failure (non-zero).

Appendix A

SUNDIALS Package Installation Procedure

The installation of any SUNDIALS package is accomplished by installing the SUNDIALS suite as a whole, according to the instructions that follow. The same procedure applies whether or not the downloaded file contains one or all solvers in SUNDIALS.

The SUNDIALS suite (or individual solvers) are distributed as compressed archives (`.tar.gz`). The name of the distribution archive is of the form *solver*`-x.y.z.tar.gz`, where *solver* is one of: `sundials`, `cvode`, `cvodes`, `arkode`, `ida`, `idas`, or `kinsol`, and `x.y.z` represents the version number (of the SUNDIALS suite or of the individual solver). To begin the installation, first uncompress and expand the sources, by issuing

```
% tar xzf solver-x.y.z.tar.gz
```

This will extract source files under a directory *solver*`-x.y.z`.

Starting with version `2.6.0` of SUNDIALS, CMake is the only supported method of installation. The explanations of the installation procedure begins with a few common observations:

- The remainder of this chapter will follow these conventions:

  solverdir is the directory *solver*`-x.y.z` created above; i.e., the directory containing the SUNDIALS sources.

  builddir is the (temporary) directory under which SUNDIALS is built.

  instdir is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory *instdir*`/include` while libraries are installed under *instdir*`/CMAKE_INSTALL_LIBDIR`, with *instdir* and `CMAKE_INSTALL_LIBDIR` specified at configuration time.

- For SUNDIALS CMake-based installation, in-source builds are prohibited; in other words, the build directory *builddir* can **not** be the same as *solverdir* and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.

- The installation directory *instdir* can **not** be the same as the source directory *solverdir*.

- By default, only the libraries and header files are exported to the installation directory *instdir*. If enabled by the user (with the appropriate toggle for CMake), the examples distributed with SUNDIALS will be built together with the solver libraries but the installation step will result in exporting (by default in a subdirectory of the installation directory) the example sources and sample outputs together with automatically generated configuration files that reference the *installed* SUNDIALS headers and libraries. As such, these configuration files for the SUNDIALS examples can be used as "templates" for your own problems. CMake installs `CMakeLists.txt` files

and also (as an option available only under Unix/Linux) `Makefile` files. Note this installation approach also allows the option of building the SUNDIALS examples without having to install them. (This can be used as a sanity check for the freshly built libraries.)

- Even if generation of shared libraries is enabled, only static libraries are created for the FCMIX modules. (Because of the use of fixed names for the Fortran user-provided subroutines, FCMIX shared libraries would result in "undefined symbol" errors at link time.)

A.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Makefiles, as well as KDevelop, Visual Studio, and (Apple) XCode project files from the same configuration file. In addition, CMake also provides a GUI front end and which allows an interactive build and installation process.

The SUNDIALS build process requires CMake version `3.1.3` or higher and a working C compiler. On Unix-like operating systems, it also requires Make (and `curses`, including its development libraries, for the GUI front end to CMake, `ccmake`), while on Windows it requires Visual Studio. CMake is continually adding new features, and the latest version can be downloaded from `http://www.cmake.org`. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use `ccmake`, while Windows users will be able to use `CMakeSetup`.

As previously noted, when using CMake to configure, build and install SUNDIALS, it is always required to use a separate build directory. While in-source builds are possible, they are explicitly prohibited by the SUNDIALS CMake scripts (one of the reasons being that, unlike autotools, CMake does not provide a `make distclean` procedure and it is therefore difficult to clean-up the source tree after an in-source build). By ensuring a separate build directory, it is an easy task for the user to clean-up all traces of the build by simply removing the build directory. CMake does generate a `make clean` which will remove files generated by the compiler and linker.

A.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The *instdir* defaults to `/usr/local` and can be changed by setting the `CMAKE_INSTALL_PREFIX` variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the `cmake` command, or from a `curses`-based GUI by using the `ccmake` command. Examples for using both methods will be presented. For the examples shown it is assumed that there is a top level SUNDIALS directory with appropriate source, build and install directories:

```
% mkdir (...)sundials/instdir
% mkdir (...)sundials/builddir
% cd (...)sundials/builddir
```

Building with the GUI

Using CMake with the GUI follows this general process:

- Select and modify values, run configure (`c` key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
  - If it is a boolean (ON/OFF) it will toggle the value
  - If it is string or file, it will allow editing of the string

  - For file and directories, the `<tab>` key can be used to complete

- Repeat until all values are set as desired and the generate option is available (`g` key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (`t` key)
- To search for a variable press `/` key, and to repeat the search, press the `n` key

To build the default configuration using the GUI, from the *builddir* enter the ccmake command and point to the *solverdir*:

```
% ccmake ../solverdir
```

The default configuration screen is shown in Figure A.1.

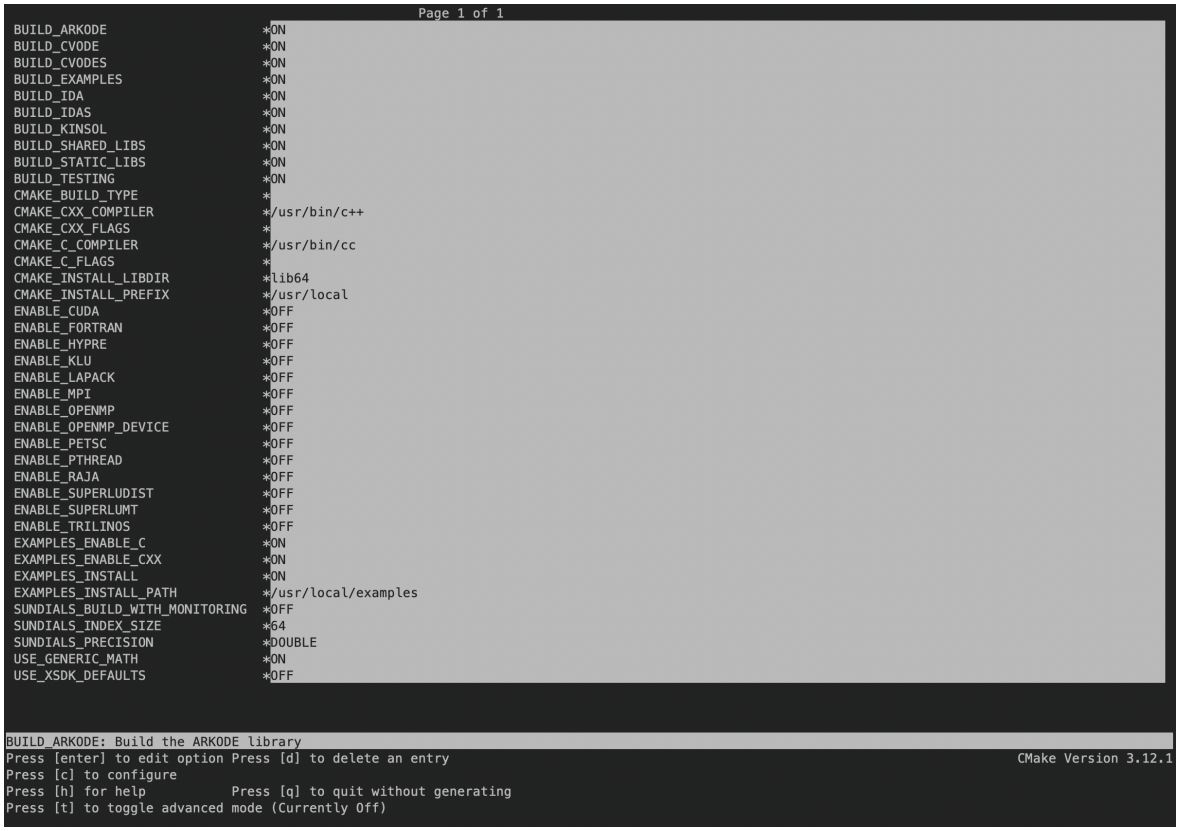

Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the `CMAKE_INSTALL_PREFIX` and the `EXAMPLES_INSTALL_PATH` as shown in figure A.2.

Pressing the (`g` key) will generate makefiles including all dependencies and all rules to build SUNDIALS on this system. Back at the command prompt, you can now run:

```
% make
```

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

```
% make install
```

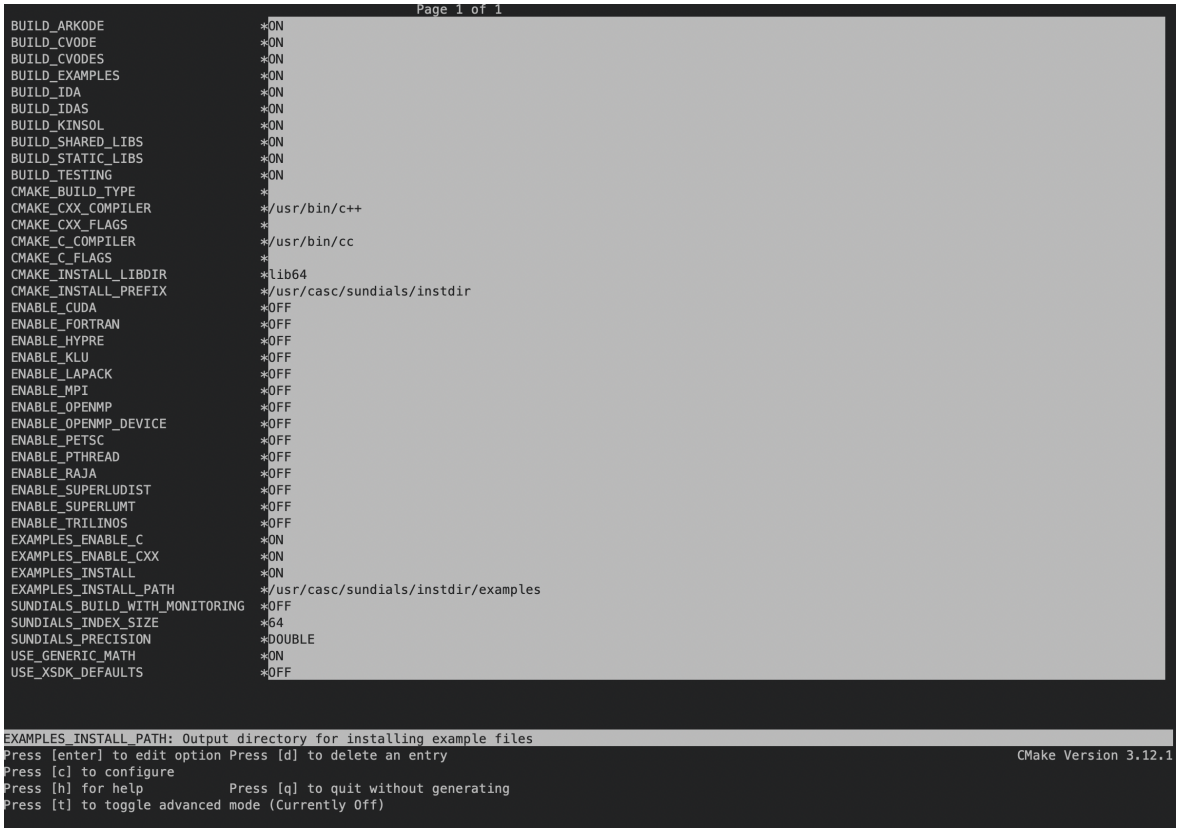

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the `cmake` command. The following will build the default configuration:

```
% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../solverdir
% make
% make install
```

A.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

`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_CXX_STANDARD` - The C++ standard to build C++ parts of SUNDIALS with.
Default: 11
Note: Options are 98, 11, 14, 17, 20. This option is on used when a C++ compiler is required.

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 LAPACK support is enabled (ENABLE_LAPACK 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

ENABLE_CUDA - Build the SUNDIALS CUDA modules.
Default: OFF

CUDA_ARCH - Specifies the CUDA architecture to compile for.
Default: sm_30

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 ENABLE_TRILINOS 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 examples
Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F2003 - Build the SUNDIALS Fortran2003 examples
Default: ON (if BUILD_FORTRAN_MODULE_INTERFACE 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

BUILD_FORTRAN_MODULE_INTERFACE - Enable Fortran-C support via the Fortran 2003 interfaces
Default: OFF

ENABLE_HYPRE - 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

ENABLE_KLU - 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

ENABLE_LAPACK - Enable LAPACK support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in A.1.4.

LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

ENABLE_MPI - 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 (ENABLE_MPI 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 ENABLE_MPI.

MPI_Fortran_COMPILER - mpif77 or mpif90 program
Default:
Note: This option is triggered only if MPI is enabled (ENABLE_MPI is ON) and Fortran-C support is enabled (F77_INTERFACE_ENABLE or BUILD_FORTRAN_MODULE_INTERFACE is ON).

MPIEXEC_EXECUTABLE - Specify the executable for running MPI programs
Default: mpirun
Note: This option is triggered only if MPI is enabled (ENABLE_MPI is ON).

ENABLE_OPENMP - 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

OPENMP_DEVICE_WORKS - **advanced option** - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.
Default: OFF

ENABLE_PETSC - Enable PETSc support
Default: OFF
Note: See additional information on building with PETSc enabled in **??**.

PETSC_DIR - Path to PETSc installation
Default:

PETSC_LIBRARIES - **advanced option** - Semi-colon separated list of PETSc link libraries. Unless provided by the user, this is autopopulated based on the PETSc installation found in PETSC_DIR.
Default:

PETSC_INCLUDES - **advanced option** - Semi-colon separated list of PETSc include directories. Unless provided by the user, this is autopopulated based on the PETSc installation found in PETSC_DIR.
Default:

ENABLE_PTHREAD - Enable Pthreads support (build the Pthreads NVECTOR).
Default: OFF

ENABLE_RAJA - Enable RAJA support.
Default: OFF
Note: You need to enable CUDA or HIP in order to build the RAJA vector module.

SUNDIALS_RAJA_BACKENDS - If building SUNDIALS with RAJA support, this sets the RAJA backend to target. Values supported are CUDA and HIP.
Default: CUDA

ENABLE_SUPERLUDIST - 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.

ENABLE_SUPERLUMT - 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_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_MT

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP
Default: Pthread

ENABLE_SYCL - Enable SYCL support.
Default: OFF
Note: At present the only supported SYCL compiler is the DPC++ (Intel oneAPI) compiler. CMake does not currently support autodetection of SYCL compilers and CMAKE_CXX_COMPILER must be set to a valid SYCL compiler i.e., dpcpp in order to build with SYCL support.

ENABLE_TRILINOS - 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 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_CXX_FLAGS if USE_XSDK_DEFAULTS=ON.
Note: Is is recommended to use the same flags that were used to build the Trilinos library.

SUNDIALS_BUILD_WITH_MONITORING - Build SUNDIALS with capabilties for fine-grained monitoring of solver progress and statistics. This is primarily useful for debugging.
Default: OFF
Note: Building with monitoring may result in minor performance degradation even if monitoring is not utilized.

SUNDIALS_BUILD_PACKAGE_FUSED_KERNELS - Build specialized fused kernels inside CVODE.
Default: OFF
Note: This option is currently only available when building with CUDA_ENABLE = ON. Building with fused kernels requires linking to either libsundials_cvode_fused_cuda.*lib* or libsundials_cvode_fused_stub where the latter provides CPU-only placeholders for the fused routines, in addition to libsundials_cvode.*lib*.

CMAKE_CXX_STANDARD - The C++ standard to build C++ parts of SUNDIALS with.
Default: 11
Note: Options are 99, 11, 14, 17. This option only used when a C++ compiler is required.

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

SUNDIALS_INSTALL_CMAKEDIR - Installation directory for the SUNDIALS cmake files (relative to CMAKE_INSTALL_PREFIX).
Default: CMAKE_INSTALL_PREFIX/cmake/sundials

USE_GENERIC_MATH - Use generic (stdc) math libraries
Default: ON

USE_XSDK_DEFAULTS - Enable xSDK (see for more information) default configuration settings. This sets CMAKE_BUILD_TYPE to Debug, SUNDIALS_INDEX_SIZE to 32 and SUNDIALS_PRECISION to double.
Default: OFF

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 \
> -DENABLE_MPI=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 \
> -DENABLE_MPI=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 any external libraries used with SUNDIALS must also be build as a shared library or as a static library compiled with the `-fPIC` flag.

Building with LAPACK

To enable LAPACK, set the `ENABLE_LAPACK` 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 rquired for LAPACK.

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DENABLE_LAPACK=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/libblas.so;/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/solverdir
%
% make install
%
```

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 5.7.2. To enable KLU, set ENABLE_KLU 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 ENABLE_SUPERLUMT 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_LIBRARIES must be set to a semi-colon separated list of other libraries SuperLU_MT depends on. For example, if SuperLU_MT ws build with an external blas library, then include the full path to the blas library in this list. Additionally, 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 ENABLE_OPENMP or ENABLE_PTHREAD 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 6.1.1. To enable SuperLU_DIST, set ENABLE_SUPERLUDIST 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 ENABLE_PTHREAD 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 3.10.0–3.14.0. To enable PETSc, set ENABLE_PETSC to ON and then set PETSC_DIR to the path of the PETSc installation. Alternatively, a user can provide a list of include paths in PETSC_INCLUDES, and a list of complete paths to the libraries needed in PETSC_LIBRARIES.

Building with *hypre*

The *hypre* libraries are available for download from the Lawrence Livermore National Laboratory website: `http://computing.llnl.gov/projects/hypre`. SUNDIALS has been tested with *hypre* version 2.14.0–2.19.0. To enable *hypre*, set `ENABLE_HYPRE` 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.

Note: SUNDIALS must be configured so that `SUNDIALS_INDEX_SIZE` (or equivalently, `XSDK_INDEX_SIZE`) equals the precision of `HYPRE_BigInt` in the corresponding *hypre* installation.

Building with CUDA

SUNDIALS CUDA modules and examples have been tested with versions 9 through 11.0.2 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 `ENABLE_CUDA` 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 up to version 0.12.1. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set `ENABLE_CUDA` and `ENABLE_RAJA` 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 12.14.1 – 12.18.1. To enable Trilinos, set `ENABLE_TRILINOS` 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.

A.4.1 Using SUNDIALS as a Third Party Library in other CMake Projects

The make install command will also install a CMake package configuration file that other CMake projects can load to get all the information needed to build against SUNDIALS. In the consuming project's CMake code, the find_package command may be used to search for the configuration file, which will be installed to instdir/SUNDIALS_INSTALL_CMAKEDIR/SUNDIALSConfig.cmake alongside a package version file instdir/SUNDIALS_INSTALL_CMAKEDIR/SUNDIALSConfigVersion.cmake. Together these files contain all the information the consuming project needs to use SUNDIALS, including exported CMake targets. The SUNDIALS exported CMake targets follow the same naming convention as the generated library binaries, e.g. the exported target for CVODE is SUNDIALS::cvode. The CMake code snipped below shows how a consuming project might leverage the SUNDIALS package configuration file to build against SUNDIALS in their own CMake project.

```
project(MyProject)

# Set the variable SUNDIALS_DIR to the SUNDIALS instdir.
# When using the cmake CLI command, this can be done like so:
#   cmake -D SUNDIALS_DIR=/path/to/sundials/installation

find_project(SUNDIALS REQUIRED)

add_executable(myexec main.c)

# Link to SUNDIALS libraries through the exported targets.
# This is just an example, users should link to the targets appropriate
# for their use case.
target_link_libraries(myexec PUBLIC SUNDIALS::cvode SUNDIALS::nvecpetsc)
```

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 sundials/sundials_cuda_policies.hpp
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 libsundials_fnvecparallel_mod.*lib*
	Header files	nvector/nvector_parallel.h
	Module files	fnvector_parallel_mod.mod
NVECTOR_MANYVECTOR	Libraries	libsundials_nvecmanyvector.*lib* libsundials_nvecmanyvector_mod.*lib*
	Header files	nvector/nvector_manyvector.h
	Module files	fnvector_manyvector_mod.mod
NVECTOR_MPIMANYVECTOR	Libraries	libsundials_nvecmpimanyvector.*lib* libsundials_nvecmpimanyvector_mod.*lib*
	Header files	nvector/nvector_mpimanyvector.h
	Module files	fnvector_mpimanyvector_mod.mod

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NVECTOR_MPIPLUSX	Libraries	libsundials_nvecmpiplusx.*lib* libsundials_nvecmpiplusx_mod.*lib*
	Header files	nvector/nvector_mpiplusx.h
	Module files	fnvector_mpiplusx_mod.mod
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
NVECTOR_PETSC	Libraries	libsundials_nvecpetsc.*lib*
	Header files	nvector/nvector_petsc.h
NVECTOR_CUDA	Libraries	libsundials_nveccuda.*lib*
	Header files	nvector/nvector_cuda.h
NVECTOR_HIP	Libraries	libsundials_nvechip.*lib*
	Header files	nvector/nvector_hip.h
NVECTOR_RAJA	Libraries	libsundials_nveccudaraja.*lib* libsundials_nvechipraja.*lib*
	Header files	nvector/nvector_raja.h
NVECTOR_SYCL	Libraries	libsundials_nvecsycl.*lib*
	Header files	nvector/nvector_sycl.h
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

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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
SUNMATRIX_SLUNRLOC	Libraries	libsundials_sunmatrixslunrloc.*lib*
	Header files	sunmatrix/sunmatrix_slunrloc.h
SUNLINSOL_CUSPARSE	Libraries	libsundials_sunmatrixcusparse.*lib*
	Header files	sunmatrix/sunmatrix_cusparse.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.*lib* libsundials_fsunlinsolband_mod.*lib* libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module files	fsunlinsol_band_mod.mod
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.*lib* libsundials_fsunlinsoldense_mod.*lib* libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	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*

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		libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module files	fsunlinsol_pcg_mod.mod
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.*lib* libsundials_fsunlinsolspbcgs_mod.*lib* libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module files	fsunlinsol_spbcgs_mod.mod
SUNLINSOL_SPFGMR	Libraries	libsundials_sunlinsolspfgmr.*lib* libsundials_fsunlinsolspfgmr_mod.*lib* libsundials_fsunlinsolspfgmr.a
	Header files	sunlinsol/sunlinsol_spfgmr.h
	Module files	fsunlinsol_spfgmr_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr.*lib* libsundials_fsunlinsolspgmr_mod.*lib* libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.*lib* libsundials_fsunlinsolsptfqmr_mod.*lib* libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
	Module files	fsunlinsol_sptfqmr_mod.mod
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.*lib* libsundials_fsunlinsolsuperlumt.a
	Header files	sunlinsol/sunlinsol_superlumt.h
SUNLINSOL_SUPERLUDIST	Libraries	libsundials_sunlinsolsuperludist.*lib*
	Header files	sunlinsol/sunlinsol_superludist.h
SUNLINSOL_CUSOLVERSP_BATCHQR	Libraries	libsundials_sunlinsolcusolversp.*lib*
	Header files	sunlinsol/sunlinsol_cusolverp_batchqr.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*
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		libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod.*lib*	
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h	
	Module files	fsunnonlinsol_fixedpoint_mod.mod	
SUNNONLINSOL_PETSCSNES	Libraries	libsundials_sunnonlinsolpetscsnes.*lib*	
	Header files	sunnonlinsol/sunnonlinsol_petscsnes.h	
CVODE	Libraries	libsundials_cvode.*lib* libsundials_fcvode.a libsundials_fcvode_mod.*lib*	
	Header files	cvode/cvode.h cvode/cvode_direct.h cvode/cvode_spils.h cvode/cvode_bbdpre.h	cvode/cvode_impl.h cvode/cvode_ls.h cvode/cvode_bandpre.h
	Module files	fcvode_mod.mod	
CVODES	Libraries	libsundials_cvodes.*lib* libsundials_fcvodes_mod.*lib*	
	Header files	cvodes/cvodes.h cvodes/cvodes_direct.h cvodes/cvodes_spils.h cvodes/cvodes_bbdpre.h	cvodes/cvodes_impl.h cvodes/cvodes_ls.h cvodes/cvodes_bandpre.h
	Module files	fcvodes_mod.mod	
ARKODE	Libraries	libsundials_arkode.*lib* libsundials_farkode.a libsundials_farkode_mod.*lib*	
	Header files	arkode/arkode.h arkode/arkode_ls.h arkode/arkode_bbdpre.h	arkode/arkode_impl.h arkode/arkode_bandpre.h
	Module files	farkode_mod.mod farkode_erkstep_mod.mod	farkode_arkstep_mod.mod farkode_mristep_mod.mod
IDA	Libraries	libsundials_ida.*lib* libsundials_fida.a libsundials_fida_mod.*lib*	
	Header files	ida/ida.h ida/ida_direct.h ida/ida_spils.h	ida/ida_impl.h ida/ida_ls.h ida/ida_bbdpre.h
	Module files	fida_mod.mod	

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IDAS	Libraries	libsundials_idas.*lib* libsundials_fidas_mod.*lib*	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_spils.h	idas/idas_impl.h idas/idas_ls.h idas/idas_bbdpre.h
	Module files	fidas_mod.mod	
KINSOL	Libraries	libsundials_kinsol.*lib* libsundials_fkinsol.a libsundials_fkinsol_mod.*lib*	
	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_spils.h	kinsol/kinsol_impl.h kinsol/kinsol_ls.h kinsol/kinsol_bbdpre.h
	Module files	fkinsol_mod.mod	

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.

Appendix C

SUNDIALS Release History

Table C.1: Release History

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Jan 2021	5.7.0	4.7.0	5.7.0	5.7.0	5.7.0	4.7.0	5.7.0
Dec 2020	5.6.1	4.6.1	5.6.1	5.6.1	5.6.1	4.6.1	5.6.1
Dec 2020	5.6.0	4.6.0	5.6.0	5.6.0	5.6.0	4.6.0	5.6.0
Oct 2020	5.5.0	4.5.0	5.5.0	5.5.0	5.5.0	4.5.0	5.5.0
Sep 2020	5.4.0	4.4.0	5.4.0	5.4.0	5.4.0	4.4.0	5.4.0
May 2020	5.3.0	4.3.0	5.3.0	5.3.0	5.3.0	4.3.0	5.3.0
Mar 2020	5.2.0	4.2.0	5.2.0	5.2.0	5.2.0	4.2.0	5.2.0
Jan 2020	5.1.0	4.1.0	5.1.0	5.1.0	5.1.0	4.1.0	5.1.0
Oct 2019	5.0.0	4.0.0	5.0.0	5.0.0	5.0.0	4.0.0	5.0.0
Feb 2019	4.1.0	3.1.0	4.1.0	4.1.0	4.1.0	3.1.0	4.1.0
Jan 2019	4.0.2	3.0.2	4.0.2	4.0.2	4.0.2	3.0.2	4.0.2
Dec 2018	4.0.1	3.0.1	4.0.1	4.0.1	4.0.1	3.0.1	4.0.1
Dec 2018	4.0.0	3.0.0	4.0.0	4.0.0	4.0.0	3.0.0	4.0.0
Oct 2018	3.2.1	2.2.1	3.2.1	3.2.1	3.2.1	2.2.1	3.2.1
Sep 2018	3.2.0	2.2.0	3.2.0	3.2.0	3.2.0	2.2.0	3.2.0
Jul 2018	3.1.2	2.1.2	3.1.2	3.1.2	3.1.2	2.1.2	3.1.2
May 2018	3.1.1	2.1.1	3.1.1	3.1.1	3.1.1	2.1.1	3.1.1
Nov 2017	3.1.0	2.1.0	3.1.0	3.1.0	3.1.0	2.1.0	3.1.0
Sep 2017	3.0.0	2.0.0	3.0.0	3.0.0	3.0.0	2.0.0	3.0.0
Sep 2016	2.7.0	1.1.0	2.9.0	2.9.0	2.9.0	1.3.0	2.9.0
Aug 2015	2.6.2	1.0.2	2.8.2	2.8.2	2.8.2	1.2.2	2.8.2
Mar 2015	2.6.1	1.0.1	2.8.1	2.8.1	2.8.1	1.2.1	2.8.1
Mar 2015	2.6.0	1.0.0	2.8.0	2.8.0	2.8.0	1.2.0	2.8.0

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Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Mar 2012	2.5.0	–	2.7.0	2.7.0	2.7.0	1.1.0	2.7.0
May 2009	2.4.0	–	2.6.0	2.6.0	2.6.0	1.0.0	2.6.0
Nov 2006	2.3.0	–	2.5.0	2.5.0	2.5.0	–	2.5.0
Mar 2006	2.2.0	–	2.4.0	2.4.0	2.4.0	–	2.4.0
May 2005	2.1.1	–	2.3.0	2.3.0	2.3.0	–	2.3.0
Apr 2005	2.1.0	–	2.3.0	2.2.0	2.3.0	–	2.3.0
Mar 2005	2.0.2	–	2.2.2	2.1.2	2.2.2	–	2.2.2
Jan 2005	2.0.1	–	2.2.1	2.1.1	2.2.1	–	2.2.1
Dec 2004	2.0.0	–	2.2.0	2.1.0	2.2.0	–	2.2.0
Jul 2002	1.0.0	–	2.0.0	1.0.0	2.0.0	–	2.0.0
Mar 2002	–	–	1.0.0[3]	–	–	–	–
Feb 1999	–	–	–	–	1.0.0[4]	–	–
Aug 1998	–	–	–	–	–	–	1.0.0[5]
Jul 1997	–	–	1.0.0[2]	–	–	–	–
Sep 1994	–	–	1.0.0[1]	–	–	–	–

[1]CVODE written, [2]PVODE written, [3]CVODE and PVODE combined, [4]IDA written, [5]KINSOL written

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