User Documentation for IDAS v4.7.0
(SUNDIALS v5.7.0)

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Chapter 1

Introduction

IDAS is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [35]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities, CVODES and IDAS.

IDAS is a general purpose solver for the initial value problem (IVP) for systems of differential-algebraic equations (DAEs). The name IDAS stands for Implicit Differential-Algebraic solver with Sensitivity capabilities. IDAS is an extension of the IDA solver within SUNDIALS, itself based on DASPK [14, 15]; however, like all SUNDIALS solvers, IDAS is written in ANSI-standard C rather than FORTRAN77. Its most notable features are that, (1) in the solution of the underlying nonlinear system at each time step, it offers a choice of Newton/direct methods and a choice of Inexact Newton/Krylov (iterative) methods; (2) it is written in a *data-independent* manner in that it acts on generic vectors and matrices without any assumptions on the underlying organization of the data; and (3) it provides a flexible, extensible framework for sensitivity analysis, using either *forward* or *adjoint* methods. Thus IDAS shares significant modules previously written within CASC at LLNL to support the ordinary differential equation (ODE) solvers CVODE [36, 22] and PVODE [18, 19], the DAE solver IDA [39] on which IDAS is based, the sensitivity-enabled ODE solver CVODES [37, 53], and also the nonlinear system solver KINSOL [23].

At present, IDAS may utilize a variety of Krylov methods provided in SUNDIALS that can be used in conjuction with Newton iteration: these include the GMRES (Generalized Minimal RESidual) [52], FGMRES (Flexible Generalized Minimum RESidual) [51], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [56], TFQMR (Transpose-Free Quasi-Minimal Residual) [30], and PCG (Preconditioned Conjugate Gradient) [32] linear iterative methods. As Krylov methods, these require little matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner matrix, and, for most problems, preconditioning is essential for an efficient solution.

For very large DAE systems, the Krylov methods are preferable over direct linear solver methods, and are often the only feasible choice. Among the Krylov methods in SUNDIALS, we recommend GMRES as the best overall choice. However, users are encouraged to compare all options, especially if encountering convergence failures with GMRES. Bi-CGFStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size. FGMRES has an advantage in that it is designed to support preconditioners that vary between iterations (e.g. iterative methods). PCG exhibits rapid convergence and minimal workspace vectors, but only works for symmetric linear systems.

IDAS is written with a functionality that is a superset of that of IDA. Sensitivity analysis capabilities, both forward and adjoint, have been added to the main integrator. Enabling forward sensitivity computations in IDAS will result in the code integrating the so-called *sensitivity equations* simultaneously with the original IVP, yielding both the solution and its sensitivity with respect to parameters in the model. Adjoint sensitivity analysis, most useful when the gradients of relatively few functionals of the solution with respect to many parameters are sought, involves integration of the original IVP

forward in time followed by the integration of the so-called *adjoint equations* backward in time. IDAS provides the infrastructure needed to integrate any final-condition ODE dependent on the solution of the original IVP (in particular the adjoint system).

There are several motivations for choosing the C language for IDAS. First, a general movement away from FORTRAN and toward C in scientific computing was apparent. Second, the pointer, structure, and dynamic memory allocation features in C are extremely useful in software of this complexity, with the great variety of method options offered. Finally, we prefer C over C++ for IDAS because of the wider availability of C compilers, the potentially greater efficiency of C, and the greater ease of interfacing the solver to applications written in extended FORTRAN.

1.1   Changes from previous versions

Changes in v4.7.0

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 9.12 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 11.13 for more details.

Changes in v4.6.1

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 v4.6.0

A new NVECTOR implementation based on the AMD ROCm HIP platform has been added. This vector can target NVIDIA or AMD GPUs. See 9.10 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 v4.5.0

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 v4.4.0

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`.

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

This change may cause an error in existing user code. The `IDASolveF` function for forward integration with checkpointing is now subject to a restriction on the number of time steps allowed to reach the output time. This is the same restriction applied to the `IDASolve` function. The default maximum number of steps is 500, but this may be changed using the `IDASetMaxNumSteps` function. This change fixes a bug that could cause an infinite loop in the `IDASolveF` function.

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`, or `IDAGetSensNumNonlinSolvIters`, the cumulative number of failures with `IDAGetNumNonlinSolvConvFails` or `IDAGetSensNumNonlinSolvConvFails`, or both with `IDAGetNonlinSolvStats` or `IDAGetSensNonlinSolvStats`.

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 8.1,13.1, 9.9 and 9.11 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 v4.3.0

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 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 functions `IDASetJacTimesResFn` and `IDASetJacTimesResFnB` to specify an alternative residual function for computing Jacobian-vector products with the internal difference quotient approximation.

Changes in v4.2.0

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.

Fixed a memory leak from not deallocating the `atolSmin0` and `atolQSmin0` arrays.

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 functions `IDASetLinearSolutionScaling` and `IDASetLinearSolutionScalingB` were 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 v4.1.0

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

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

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

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

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

Changes in v4.0.0

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 §9.1.6 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 §9.15 and §9.16 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 §9.1.4 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 §9.17 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 §9.9.1 for more details.

- Added new Fortran 2003 interfaces for most NVECTOR modules. See Chapter 9 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 §9.1.6 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 §10.1.2 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 §10.1.1 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 §10.1.3 for more details.

- A new SUNMATRIX (and SUNLINSOL) implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS. See §10.6 for more details.

- Added new Fortran 2003 interfaces for most SUNMATRIX modules. See Chapter 10 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 §11.3 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 §11.10 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 §11.12 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 §11.9.2 for more details.

- Added new Fortran 2003 interfaces for most SUNLINSOL modules. See Chapter 11 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 §12.1.8 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 SUN-NONLINSOL 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 §12.2 and for more details on the API functions see Chapter 12.

- Added a new SUNNONLINSOL implementation, SUNNONLINSOL_PETSCSNES, which interfaces to the PETSc SNES nonlinear solver API. See §12.4 for more details.

- Added new Fortran 2003 interfaces for most SUNNONLINSOL modules. See Chapter 12 for more details on how to use the interfaces.

IDAS changes

- A bug was fixed in the IDAS linear solver interface where an incorrect Jacobian-vector product increment was used with iterative solvers other than SUNLINSOL_SPGMR and SUNLINSOL_SPFGMR.

- Fixed a bug where the `IDASolveF` function would not return a root in `IDA_NORMAL_STEP` mode if the root occurred after the desired output time.

- Fixed a bug where the `IDASolveF` function would return the wrong flag under certrain cirumstances.

- Fixed a bug in `IDAQuadReInitB` where an incorrect memory structure was passed to `IDAQuadReInit`.

- 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, IDAS 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`, `IDAComputeCurrentYp`, `IDAGetCurrentYSens`, `IDAGetCurrentYpSens`, `IDAComputeCurrentYSens`, and `IDAComputeCurrentYpSens`, which may be useful to users who choose to provide their own nonlinear solver implementations.

- Added a Fortran 2003 interface to IDAS. See Chapter 7 for more details.

Changes in v3.1.0

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 `idas_impl.h` is no longer installed. This means users who are directly manipulating the `IDAMem` structure will need to update their code to use IDAS's public API.

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

Changes in v3.0.2

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 IDAS library, `libsundials_idas`.

Changes in v3.0.1

No changes were made in this release.

Changes in v3.0.0

IDAS' previous direct and iterative linear solver interfaces, IDADLS and IDASPILS, have been merged into a single unified linear solver interface, IDALS, to support any valid SUNLINSOL module. This includes the "DIRECT" and "ITERATIVE" types as well as the new "MATRIX_ITERATIVE" type. Details regarding how IDALS utilizes linear solvers of each type as well as discussion regarding intended use cases for user-supplied SUNLINSOL implementations are included in Chapter 11. All IDAS example programs and the standalone linear solver examples have been updated to use the unified linear solver interface.

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

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

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

SUNDIALS integrators have been updated to utilize generic nonlinear solver modules defined through the SUNNONLINSOL API. This API will ease the addition of new nonlinear solver options and allow for external or user-supplied nonlinear solvers. The SUNNONLINSOL API and SUNDIALS provided modules are described in Chapter 12 and follow the same object oriented design and implementation used by the NVECTOR, SUNMATRIX, and SUNLINSOL modules. Currently two SUNNONLINSOL implementations are provided, SUNNONLINSOL_NEWTON and SUNNONLINSOL_FIXEDPOINT. These replicate the previous integrator specific implementations of a Newton iteration and a fixed-point iteration (previously referred to as a functional iteration), respectively. Note the SUNNONLINSOL_FIXEDPOINT module can optionally utilize Anderson's method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all IDAS example programs have been updated to use generic SUNNONLINSOL modules.

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

Three fused vector operations and seven vector array operations have been added to the NVECTOR API. These *optional* operations are disabled by default and may be activated by calling vector specific routines after creating an NVECTOR (see Chapter 9 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 §9.13 for more details.

Changes in v2.2.1

The changes in this minor release include the following:

- Fixed a bug in the CUDA NVECTOR where the N_VInvTest operation could write beyond the allocated vector data.

- Fixed library installation path for multiarch systems. This fix changes the default library installation path to CMAKE_INSTALL_PREFIX/CMAKE_INSTALL_LIBDIR from CMAKE_INSTALL_PREFIX/lib. CMAKE_INSTALL_LIBDIR is automatically set, but is available as a CMake option that can modified.

Changes in v2.2.0

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

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

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

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

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

Several changes were made to the build system:

- CMake 3.1.3 is now the minimum required CMake version.

- Deprecate the behavior of the `SUNDIALS_INDEX_TYPE` CMake option and added the `SUNDIALS_INDEX_SIZE` CMake option to select the `sunindextype` integer size.

- The native CMake FindMPI module is now used to locate an MPI installation.

- If MPI is enabled and MPI compiler wrappers are not set, the build system will check if `CMAKE_<language>_COMPILER` can compile MPI programs before trying to locate and use an MPI installation.

- The previous options for setting MPI compiler wrappers and the executable for running MPI programs have been have been deprecated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPI_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.

- When a Fortran name-mangling scheme is needed (e.g., `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 v2.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using rpath by default to locate shared libraries on OSX.

- Fixed Windows specific problem where `sunindextype` was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows `sunindextype` is now defined as the MSVC basic type `__int64`.

- Added sparse SUNMatrix "Reallocate" routine to allow specification of the nonzero storage.

- Updated the KLU SUNLINSOL module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.

- Updated the "ScaleAdd" and "ScaleAddI" implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum $I + \gamma J$ manually (with zero entries if needed).

- Changed the LICENSE install path to `instdir/include/sundials`.

Changes in v2.1.1

The changes in this minor release include the following:

- Fixed a potential memory leak in the SPGMR and SPFGMR linear solvers: if "Initialize" was called multiple times then the solver memory was reallocated (without being freed).

- Updated KLU SUNLinearSolver module to use a `typedef` for the precision-specific solve function to be used (to avoid compiler warnings).

- Added missing typecasts for some (`void*`) pointers (again, to avoid compiler warnings).

- Bugfix in `sunmatrix_sparse.c` where we had used `int` instead of `sunindextype` in one location.

- Added missing `#include <stdio.h>` in NVECTOR and SUNMATRIX header files.

- Added missing prototype for `IDASpilsGetNumJTSetupEvals`.

- Fixed an indexing bug in the CUDA NVECTOR implementation of `N_VWrmsNormMask` and revised the RAJA NVECTOR implementation of `N_VWrmsNormMask` to work with mask arrays using values other than zero or one. Replaced `double` with `realtype` in the RAJA vector test functions.

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

Changes in v2.1.0

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

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

Changes in v2.0.0

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

- Added generic SUNMATRIX module with three provided implementations: dense, banded and sparse. These replicate previous SUNDIALS Dls and Sls matrix structures in a single object-oriented API.

- Added example problems demonstrating use of generic SUNMATRIX modules.

- Added generic `SUNLinearSolver` module with eleven provided implementations: SUNDIALS native dense, SUNDIALS native banded, LAPACK dense, LAPACK band, KLU, SuperLU_MT, SPGMR, SPBCGS, SPTFQMR, SPFGMR, and PCG. These replicate previous SUNDIALS generic linear solvers in a single object-oriented API.

- Added example problems demonstrating use of generic `SUNLinearSolver` modules.

- Expanded package-provided direct linear solver (Dls) interfaces and scaled, preconditioned, iterative linear solver (Spils) interfaces to utilize generic SUNMATRIX and `SUNLinearSolver` objects.

- Removed package-specific, linear solver-specific, solver modules (e.g. `CVDENSE`, `KINBAND`, `IDAKLU`, `ARKSPGMR`) since their functionality is entirely replicated by the generic Dls/Spils interfaces and `SUNLinearSolver`/`SUNMATRIX` modules. The exception is `CVDIAG`, a diagonal approximate Jacobian solver available to CVODE and CVODES.

- Converted all SUNDIALS example problems and files to utilize the new generic SUNMATRIX and `SUNLinearSolver` objects, along with updated Dls and Spils linear solver interfaces.

- Added Spils interface routines to ARKODE, CVODE, CVODES, IDA, and IDAS to allow specification of a user-provided "JTSetup" routine. This change supports users who wish to set up data structures for the user-provided Jacobian-times-vector ("JTimes") routine, and where the cost of one JTSetup setup per Newton iteration can be amortized between multiple JTimes calls.

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

All indices for data structures were updated to a new `sunindextype` that can be configured to be a 32- or 64-bit integer data index type. `sunindextype` is defined to be `int32_t` or `int64_t` when portable types are supported, otherwise it is defined as `int` or `long int`. The Fortran interfaces continue to use `long int` for indices, except for their sparse matrix interface that now uses the new `sunindextype`. This new flexible capability for index types includes interfaces to PETSc, hypre, SuperLU_MT, and KLU with either 32-bit or 64-bit capabilities depending how the user configures SUNDIALS.

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

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

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

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

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

In addition, numerous changes were made to the build system. These include the addition of separate `BLAS_ENABLE` and `BLAS_LIBRARIES` CMake variables, additional error checking during CMake configuration, minor bug fixes, and renaming CMake options to enable/disable examples for greater clarity and an added option to enable/disable Fortran 77 examples. These changes included changing `EXAMPLES_ENABLE` to `EXAMPLES_ENABLE_C`, changing `CXX_ENABLE` to `EXAMPLES_ENABLE_CXX`, changing `F90_ENABLE` to `EXAMPLES_ENABLE_F90`, and adding an `EXAMPLES_ENABLE_F77` option.

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

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

Changes in v1.3.0

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

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

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

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

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

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

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

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

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

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

Changes in v1.2.0

Two major additions were made to the linear system solvers that are available for use with the IDAS solver. First, in the serial case, an interface to the sparse direct solver KLU was added. Second, an interface to SuperLU_MT, the multi-threaded version of SuperLU, was added as a thread-parallel sparse direct solver option, to be used with the serial version of the NVECTOR module. As part of these additions, a sparse matrix (CSC format) structure was added to IDAS.

Otherwise, only relatively minor modifications were made to IDAS:

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

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

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

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

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

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

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

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

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

Changes in v1.1.0

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

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

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

1.2   Reading this User Guide

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by IDAS for the solution of initial value problems for systems of DAEs, continue with short descriptions of preconditioning (§2.2) and rootfinding (§2.3), and then give an overview of the mathematical aspects of sensitivity analysis, both forward (§2.5) and adjoint (§2.6).

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

- Chapter 4 is the main usage document for IDAS for simulation applications. It includes a complete description of the user interface for the integration of DAE initial value problems. Readers that are not interested in using IDAS for sensitivity analysis can then skip the next two chapters.

- Chapter 5 describes the usage of IDAS for forward sensitivity analysis as an extension of its IVP integration capabilities. We begin with a skeleton of the user main program, with emphasis on the steps that are required in addition to those already described in Chapter 4. Following that we provide detailed descriptions of the user-callable interface routines specific to forward sensitivity analysis and of the additonal optional user-defined routines.

- Chapter 6 describes the usage of IDAS for adjoint sensitivity analysis. We begin by describing the IDAS checkpointing implementation for interpolation of the original IVP solution during integration of the adjoint system backward in time, and with an overview of a user's main program. Following that we provide complete descriptions of the user-callable interface routines for adjoint sensitivity analysis as well as descriptions of the required additional user-defined routines.

- Chapter 9 gives a brief overview of the generic NVECTOR module shared amongst the various components of SUNDIALS, as well as details on the NVECTOR implementations provided with SUNDIALS.

- Chapter 10 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 (§10.3), a banded implementation (§10.4) and a sparse implementation (§10.5).

- Chapter 11 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 12 describes the SUNNONLINSOL API and nonlinear solver implementations shared among the various components of SUNDIALS.

- Finally, in the appendices, we provide detailed instructions for the installation of IDAS, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from IDAS functions (Appendix B).

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

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1.3.2   Additional Notice

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1.3.3   SUNDIALS Release Numbers

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

Chapter 2

Mathematical Considerations

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

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

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

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

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

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

2.1 IVP solution

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

The integration method used in IDAS is the variable-order, variable-coefficient BDF (Backward Differentiation Formula), in fixed-leading-coefficient form [11]. The method order ranges from 1 to 5, with the BDF of order q given by the multistep formula

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

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

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

By default IDAS solves (2.4) with a Newton iteration but IDAS also allows for user-defined nonlinear solvers (see Chapter 12). Each Newton iteration requires the soution of a linear system of the form

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

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

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

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

For the solution of the linear systems within the Newton iteration, IDAS provides several choices, including the option of a user-supplied linear solver module (see Chapter 11). 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 [24, 3], or the thread-enabled SuperLU_MT sparse solver library [45, 26, 9] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of IDAS],

- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver 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 IDAS, preconditioning is allowed only on the left (see §2.2). Note that the dense, band, and sparse direct linear solvers can only be used with serial and threaded vector representations.

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

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

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

In the case of a matrix-based linear solver, the default Newton iteration is a Modified Newton iteration, in that the Jacobian J is fixed (and usually out of date) throughout the nonlinear iterations, with a coefficient $\bar{\alpha}$ in place of α in J. However, in the case that a matrix-free iterative linear solver is used, the default Newton iteration is an Inexact Newton iteration, in which J is applied in a matrix-free manner, with matrix-vector products Jv obtained by either difference quotients or a user-supplied routine. In this case, the linear residual $J\Delta y + G$ is nonzero but controlled. With the default Newton iteration, the matrix J and preconditioner matrix P are updated as infrequently as possible to balance the high costs of matrix operations against other costs. Specifically, this matrix update occurs when:

- starting the problem,

- the value $\bar{\alpha}$ at the last update is such that $\alpha/\bar{\alpha} < 3/5$ or $\alpha/\bar{\alpha} > 5/3$, or

- a non-fatal convergence failure occurred with an out-of-date J or P.

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

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

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

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

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

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

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

When the Jacobian is stored using either dense or band SUNMATRIX objects, the Jacobian J defined in (2.6) can be either supplied by the user or have IDAS compute one internally by difference quotients. In the latter case, we use the approximation

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

where U is the unit roundoff, h is the current step size, and W_j is the error weight for the component y_j defined by (2.7). We note that with sparse and user-supplied SUNMATRIX objects, the Jacobian *must* be supplied by a user routine.

In the case of an iterative linear solver, if a routine for Jv is not supplied, such products are approximated by

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

where the increment $\sigma = 1/\|v\|$. 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, IDAS computes an estimate of the local truncation error, LTE, at the n-th time step, and requires this to satisfy the inequality

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- else reset $q \leftarrow q + 1$ if $T(q + 1) < T(q)$;

- leave q unchanged otherwise [then $T(q - 1) > T(q) \leq T(q + 1)$].

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

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

The value of η is adjusted such that (a) if $\eta > 2$, η is reset to 2; (b) if $\eta \leq 1$, η is restricted to $0.5 \leq \eta \leq 0.9$; and (c) if $1 < \eta < 2$ we use $\eta = 1$. Finally h is reset to $h' = \eta h$. Thus we do not increase the step size unless it can be doubled. See [11] for details.

IDAS permits the user to impose optional inequality constraints on individual components of the solution vector y. Any of the following four constraints can be imposed: $y_i > 0$, $y_i < 0$, $y_i \geq 0$, or $y_i \leq 0$. The constraint satisfaction is tested after a successful nonlinear system solution. If any constraint fails, we declare a convergence failure of the nonlinear iteration and reduce the step size. Rather than cutting the step size by some arbitrary factor, IDAS estimates a new step size h' using a linear approximation of the components in y that failed the constraint test (including a safety factor of 0.9 to cover the strict inequality case). These additional constraints are also imposed during the calculation of consistent initial conditions. 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, IDAS takes steps until a user-defined output value $t = t_{\mathrm{out}}$ is overtaken, and then computes $y(t_{\mathrm{out}})$ by interpolation. However, a "one step" mode option is available, where control returns to the calling program after each step. There are also options to force IDAS not to integrate past a given stopping point $t = t_{\mathrm{stop}}$.

2.2 Preconditioning

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

In order to improve the convergence of the Krylov iteration, the preconditioner matrix P should in some sense approximate the system matrix A. Yet at the same time, in order to be cost-effective, the matrix P should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [13] for an extensive study of preconditioners for reaction-transport systems).

Typical preconditioners used with IDAS are based on approximations to the iteration matrix of the systems involved; in other words, $P \approx \frac{\partial F}{\partial y} + \alpha \frac{\partial F}{\partial \dot{y}}$, where α is a scalar inversely proportional to the integration step size h. Because the Krylov iteration occurs within a nonlinear solver iteration

and further also within a time integration, and since each of these iterations has its own test for convergence, the preconditioner may use a very crude approximation, as long as it captures the dominant numerical feature(s) of the system. We have found that the combination of a preconditioner with the Newton-Krylov iteration, using even a fairly poor approximation to the Jacobian, can be surprisingly superior to using the same matrix without Krylov acceleration (i.e., a modified Newton iteration), as well as to using the Newton-Krylov method with no preconditioning.

2.3 Rootfinding

The IDAS solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (2.1), IDAS can also find the roots of a set of user-defined functions $g_i(t, y, \dot{y})$ that depend on t, the solution vector $y = y(t)$, and its $t-$derivative $\dot{y}(t)$. The number of these root functions is arbitrary, and if more than one g_i is found to have a root in any given interval, the various root locations are found and reported in the order that they occur on the t axis, in the direction of integration.

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

The basic scheme used is to check for sign changes of any $g_i(t)$ over each time step taken, and then (when a sign change is found) to home in on the root (or roots) with a modified secant method [33]. In addition, each time g is computed, IDAS checks to see if $g_i(t) = 0$ exactly, and if so it reports this as a root. However, if an exact zero of any g_i is found at a point t, IDAS computes g at $t + \delta$ for a small increment δ, slightly further in the direction of integration, and if any $g_i(t + \delta) = 0$ also, IDAS stops and reports an error. This way, each time IDAS takes a time step, it is guaranteed that the values of all g_i are nonzero at some past value of t, beyond which a search for roots is to be done.

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

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

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

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

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

where α a weight parameter. On the first two passes through the loop, α is set to 1, making t_{mid} the secant method value. Thereafter, α is reset according to the side of the subinterval (low vs high, i.e. toward t_{lo} vs toward t_{hi}) in which the sign change was found in the previous two passes. If the two sides were opposite, α is set to 1. If the two sides were the same, α is halved (if on the low

side) or doubled (if on the high side). The value of t_{mid} is closer to t_{lo} when $\alpha < 1$ and closer to t_{hi} when $\alpha > 1$. If the above value of t_{mid} is within $\tau/2$ of t_{lo} or t_{hi}, it is adjusted inward, such that its fractional distance from the endpoint (relative to the interval size) is between .1 and .5 (.5 being the midpoint), and the actual distance from the endpoint is at least $\tau/2$.

2.4 Pure quadrature integration

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

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

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

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

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

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

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

once the new approximation y_n is available.

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

2.5 Forward sensitivity analysis

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

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

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

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

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

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

2.5.1   Forward sensitivity methods

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

- *Staggered Direct* In this approach [21], the nonlinear system (2.4) is first solved and, once an acceptable numerical solution is obtained, the sensitivity variables at the new step are found by directly solving (2.12) after the BDF discretization is used to eliminate $\dot{s}_i$. Although the system matrix of the above linear system is based on exactly the same information as the matrix J in (2.6), it must be updated and factored at every step of the integration, in contrast to an evaluation of J which is updated only occasionally. For problems with many parameters (relative to the problem size), the staggered direct method can outperform the methods described below [44]. However, the computational cost associated with matrix updates and factorizations makes this method unattractive for problems with many more states than parameters (such as those arising from semidiscretization of PDEs) and is therefore not implemented in IDAS.

- *Simultaneous Corrector* In this method [48], the discretization is applied simultaneously to both the original equations (2.2) and the sensitivity systems (2.12) resulting in an "extended" nonlinear system $\hat{G}(\hat{y}_n) = 0$ where $\hat{y}_n = [y_n, \ldots, s_i, \ldots]$. This combined nonlinear system can be solved using a modified Newton method as in (2.5) by solving the corrector equation

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

  at each iteration, where

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

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

- *Staggered corrector* In this approach [29], as in the staggered direct method, the nonlinear system (2.4) is solved first using the Newton iteration (2.5). Then, for each sensitivity vector $\xi \equiv s_i$, a separate Newton iteration is used to solve the sensitivity system (2.12):

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

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

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

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

2.5.2 Selection of the absolute tolerances for sensitivity variables

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

2.5.3 Evaluation of the sensitivity right-hand side

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

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

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

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

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

or simultaneously:

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

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

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

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

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

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

2.5.4 Quadratures depending on forward sensitivities

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

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

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

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

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

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

2.6 Adjoint sensitivity analysis

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

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

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

In what follows, we only sketch the analysis for the sensitivity problem for both G and g. For details on the derivation see [20].

2.6.1   Sensitivity of $G(p)$

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

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

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

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

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

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

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

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

Now by requiring λ to satisfy

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

we obtain

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

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

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

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

yielding the sensitivity equation for dG/dp

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

This choice will not suffice for a Hessenberg index-2 DAE system. For a derivation of proper final conditions in such cases, see [20].

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

2.6.2   Sensitivity of $g(T, p)$

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

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

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

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

while for a Hessenberg index-2 DAE system we have

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

The corresponding adjoint equations are

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

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

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

Taking the total derivative, we obtain

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

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

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

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

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

For the regular implicit ODE case, $F_{\dot{y}}$ is invertible; thus we have $\lambda(T, T) = 0$, which leads to $\lambda_T(T) = -\dot{\lambda}(T)$. As with the final conditions for $\lambda(T)$ in (2.20), the above selection for $\lambda_T(T)$ is not sufficient for index-two Hessenberg DAEs (see [20] for details).

2.6.3 Checkpointing scheme

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

However, especially for large-scale problems and long integration intervals, the number and size of the vectors y and $\dot{y}$ that would need to be stored make this approach computationally intractable. Thus, IDAS settles for a compromise between storage space and execution time by implementing a so-called *checkpointing scheme.* At the cost of at most one additional forward integration, this approach offers the best possible estimate of memory requirements for adjoint sensitivity analysis. To begin with, based on the problem size N and the available memory, the user decides on the number N_d of data pairs $(y, \dot{y})$ if cubic Hermite interpolation is selected, or on the number N_d of y vectors in the case of variable-degree polynomial interpolation, that can be kept in memory for the purpose of interpolation. Then, during the first forward integration stage, after every N_d integration steps a
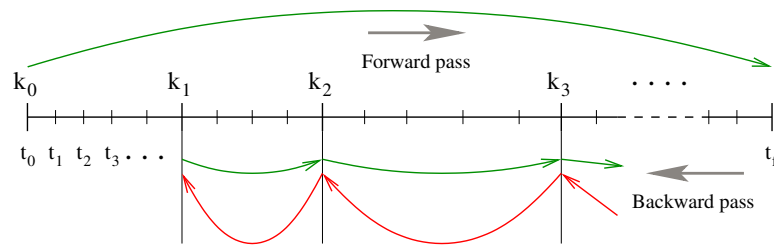
Figure 2.1: Illustration of the checkpointing algorithm for generation of the forward solution during the integration of the adjoint system.

checkpoint is formed by saving enough information (either in memory or on disk) to allow for a hot restart, that is a restart which will exactly reproduce the forward integration. In order to avoid storing Jacobian-related data at each checkpoint, a reevaluation of the iteration matrix is forced before each checkpoint. At the end of this stage, we are left with N_c checkpoints, including one at t_0. During the backward integration stage, the adjoint variables are integrated backwards from T to t_0, going from one checkpoint to the previous one. The backward integration from checkpoint $i+1$ to checkpoint i is preceded by a forward integration from i to $i+1$ during which the N_d vectors y (and, if necessary $\dot{y}$) are generated and stored in memory for interpolation[1]

This approach transfers the uncertainty in the number of integration steps in the forward integration phase to uncertainty in the final number of checkpoints. However, N_c is much smaller than the number of steps taken during the forward integration, and there is no major penalty for writing/reading the checkpoint data to/from a temporary file. Note that, at the end of the first forward integration stage, interpolation data are available from the last checkpoint to the end of the interval of integration. If no checkpoints are necessary (N_d is larger than the number of integration steps taken in the solution of (2.2)), the total cost of an adjoint sensitivity computation can be as low as one forward plus one backward integration. In addition, IDAS provides the capability of reusing a set of checkpoints for multiple backward integrations, thus allowing for efficient computation of gradients of several functionals (2.17).

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

2.7 Second-order sensitivity analysis

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

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

---

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

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

[2]For the sake of simplifity in presentation, we do not include explicit dependencies of g on time t or parameters p. Moreover, we only consider the case in which the dependency of the original DAE (2.2) on the parameters p is through its initial conditions only. For details on the derivation in the general case, see [49].

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

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

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

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

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

As an illustration[3], consider the ODE problem

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

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

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

where λ and μ are solutions of

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

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

Therefore (and this is also valid for the DAE case), the cost of computing the Hessian-vector product is roughly that of two forward and two backward integrations of a system of DAEs of size N. For more details, including the corresponding formulas for a pointwise model functional output, see the work by Ozyurt and Barton [49] who discuss this problem for ODE initial value problems. As far as we know, there is no published equivalent work on DAE problems. However, the derivations given in [49] for ODE problems can be extended to DAEs with some careful consideration given to the derivation of proper final conditions on the adjoint systems, following the ideas presented in [20].

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

- the integration of multiple backward problems depending on the same underlying forward problem (2.2), and

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

---

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

Chapter 3

Code Organization

3.1 SUNDIALS organization

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

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Figures 3.1 and 3.2). The
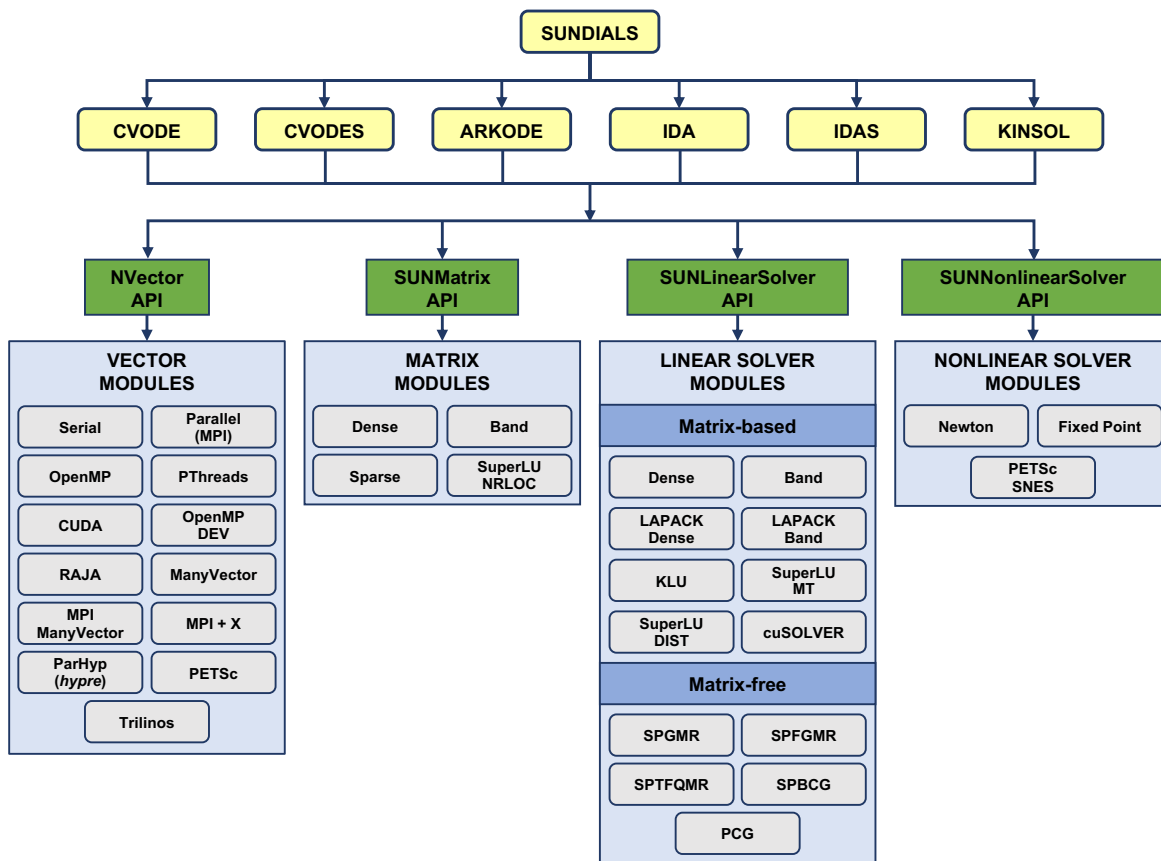
Figure 3.1: High-level diagram of the SUNDIALS suite.
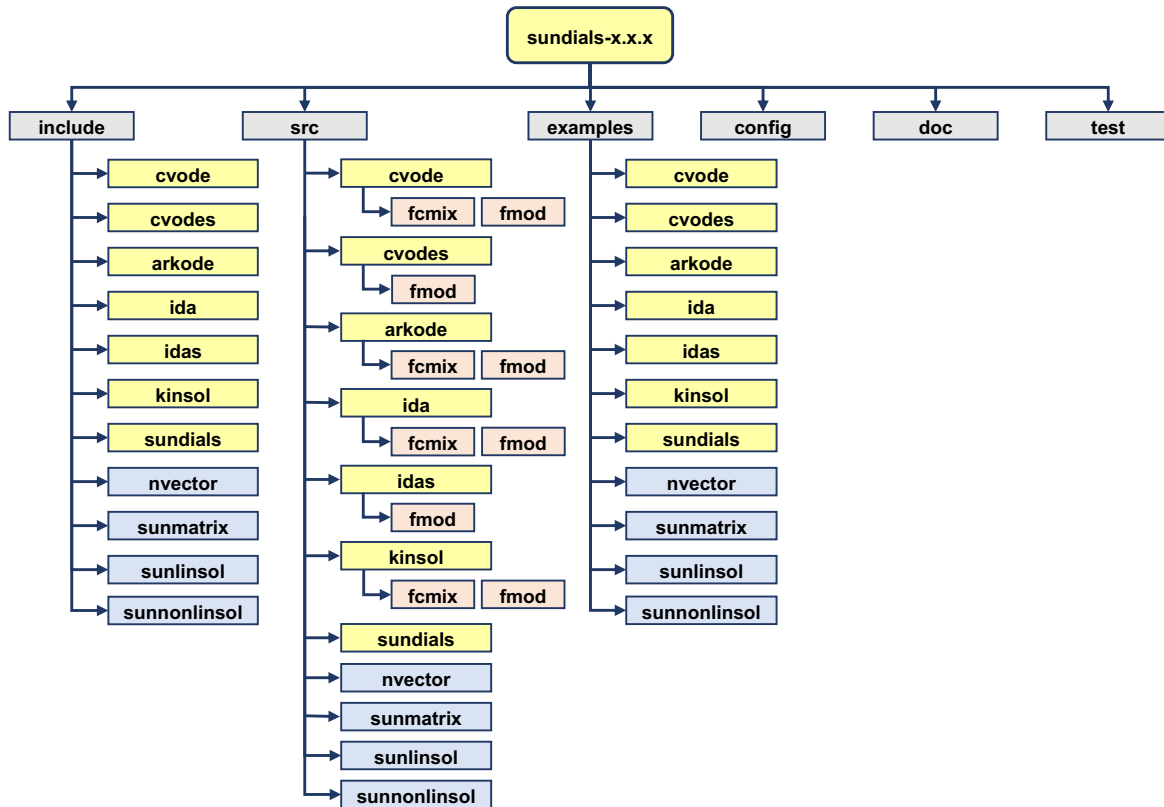
Figure 3.2: Directory structure of the SUNDIALS source tree.

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 $Mdy/dt = f_1(t, y) + f_2(t, y)$ 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 IDAS organization

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

The overall organization of the IDAS package is shown in Figure 3.3. The central integration module, implemented in the files `idas.h`, `idas_impl.h`, and `idas.c`, deals with the evaluation of
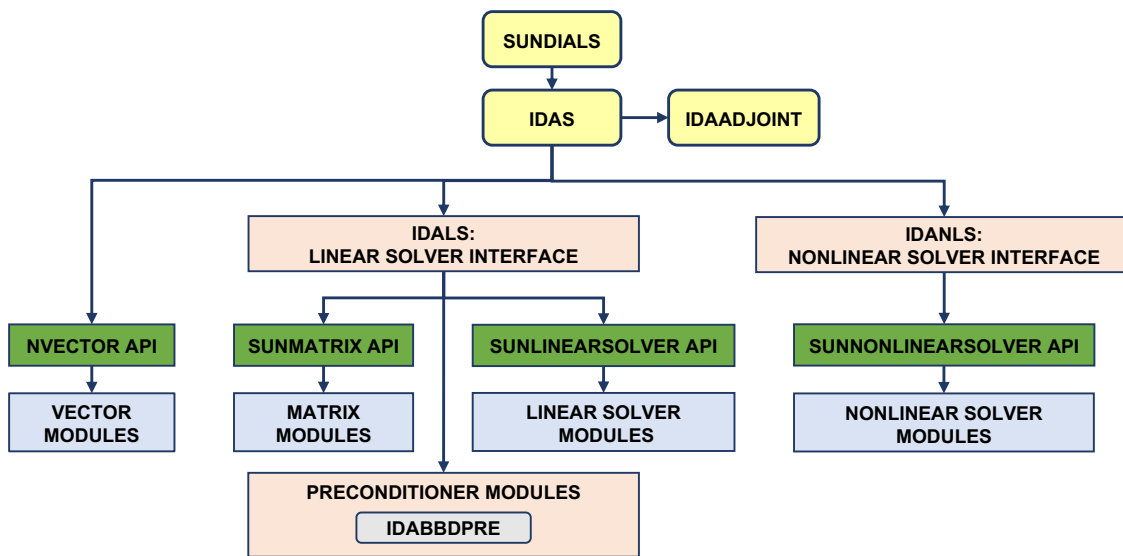
Figure 3.3: Overall structure diagram of the IDAS package. Modules specific to IDAS begin with "IDA" (IDALS, IDANLS, and IDABBDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver modules (see Figure 3.1).

integration coefficients, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues.

IDAS utilizes generic linear and nonlinear solver modules defined by the SUNLINSOL API (see Chapter 11) and SUNNONLINSOL API (see Chapter 12) respectively. As such, IDAS has no knowledge of the method being used to solve the linear and nonlinear systems that arise in each time step. For any given user problem, there exists a single nonlinear solver interface and, if necessary, one of the linear system solver interfaces is specified, and invoked as needed during the integration. While SUN-DIALS includes a fixed-point nonlinear solver module, it is not currently supported in IDAS (note the fixed-point module is listed in Figure 3.1 but not Figure 3.3).

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

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

IDAS now has a single unified linear solver interface, IDALS, supporting both direct and iterative linear solvers built using the generic SUNLINSOL API (see Chapter 11). These solvers may utilize a SUNMATRIX object (see Chapter 10) for storing Jacobian information, or they may be matrix-free. Since IDAS can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to IDAS will expand as new SUNLINSOL modules are developed.

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

For users employing matrix-free iterative linear solvers, IDALS includes an algorithm for the approx-

imation 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 IDAS, offer considerable assistance in building preconditioners.

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

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

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

Chapter 4

Using IDAS for IVP Solution

This chapter is concerned with the use of IDAS for the integration of DAEs in a C language setting. The following sections treat the header files, the layout of the user's main program, description of the IDAS user-callable functions, and description of user-supplied functions. This usage is essentially equivalent to using IDA [39].

The sample programs described in the companion document [54] may also be helpful. Those codes may be used as templates (with the removal of some lines involved in testing), and are included in the IDAS package.

Users with applications written in FORTRAN should see Chapter **??**, 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 10) and each SUNLINSOL module (Chapter 11). 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 10 and 11 to verify compatibility between these modules. In addition to that documentation, we note that the preconditioner module IDABBDPRE can only be used with NVECTOR_PARALLEL. It is not recommended to use a threaded vector module with SuperLU_MT unless it is the NVECTOR_OPENMP module, and SuperLU_MT is also compiled with OpenMP.

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

4.1   Access to library and header files

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

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

- *libdir*/`libsundials_idas.`*lib*,

- *libdir*/`libsundials_nvec*.`*lib*,

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

- *incdir*/`include/idas`

- *incdir*/`include/sundials`

- *incdir*/`include/nvector`

- *incdir*/include/sunmatrix

- *incdir*/include/sunlinsol

- *incdir*/include/sunnonlinsol

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

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

4.2   Data types

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

4.2.1   Floating point types

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

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

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

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

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

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:

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

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

The calling program must also include an NVECTOR implementation header file, of the form `nvector/nvector_***.h`. See Chapter 9 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 12 for more information). This file in turn includes the header file `sundials_nonlinearsolver.h` which defines the abstract `SUNNonlinearSolver` data type.

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

- Direct linear solvers:
    - `sunlinsol/sunlinsol_dense.h`, which is used with the dense linear solver module, SUN-LINSOL_DENSE;
    - `sunlinsol/sunlinsol_band.h`, which is used with the banded linear solver module, SUN-LINSOL_BAND;
    - `sunlinsol/sunlinsol_lapackdense.h`, which is used with the LAPACK dense linear solver module, SUNLINSOL_LAPACKDENSE;
    - `sunlinsol/sunlinsol_lapackband.h`, which is used with the LAPACK banded linear solver module, SUNLINSOL_LAPACKBAND;
    - `sunlinsol/sunlinsol_klu.h`, which is used with the KLU sparse linear solver module, SUNLINSOL_KLU;
    - `sunlinsol/sunlinsol_superlumt.h`, which is used with the SUPERLUMT sparse linear solver module, SUNLINSOL_SUPERLUMT;

- Iterative linear solvers:

  - `sunlinsol/sunlinsol_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver module, SUNLINSOL_SPGMR;

  - `sunlinsol/sunlinsol_spfgmr.h`, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, SUNLINSOL_SPFGMR;

  - `sunlinsol/sunlinsol_spbcgs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, SUNLINSOL_SPBCGS;

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

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

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

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

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

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

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the `idasFoodWeb_kry_p` example (see [54]), 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 9, 10, 11, and 12 for the specific name of the function to be called or macro to be referenced.

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

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

2. **Set problem dimensions etc.**

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

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

3. **Set vectors of initial values**

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

   For native SUNDIALS vector implementations (except the CUDA and RAJA-based ones), use a call of the form `y0 = N_VMake_***(..., ydata)` if the `realtype` array `ydata` containing the initial values of y already exists. Otherwise, create a new vector by making a call of the form `y0 =`

N_VNew_***(...), and then set its elements by accessing the underlying data with a call of the form ydata = N_VGetArrayPointer(y0). See §9.3-9.6 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 §9.7 and §9.8 for details.

If using either the CUDA- or RAJA-based vector implementations use a call of the form y0 = N_VMake_***(..., c) where c is a pointer to a suncudavec or sunrajavec vector class if this class already exists. Otherwise, create a new vector by making a call of the form y0 = N_VNew_***(...), and then set its elements by accessing the underlying data where it is located with a call of the form N_VGetDeviceArrayPointer_*** or N_VGetHostArrayPointer_***. Note that the vector class will allocate memory on both the host and device when instantiated. See §9.9-9.11 for details.

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

4. **Create IDAS object**

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

5. **Initialize IDAS solver**

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

6. **Specify integration tolerances**

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

7. **Create matrix object**

If a nonlinear solver requiring a linear solver will be used (e.g., the default Newton iteration) and the linear solver will be a matrix-based linear solver, then a template Jacobian matrix must be created by 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 11.

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 11 for details.

10. **Attach linear solver module**

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

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

11. **Set optional inputs**

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

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

    If using a non-default nonlinear solver (see §4.5.4), then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular SUNNONLINSOL implementation (e.g., `NLS = SUNNonlinSol_***(...);` where `***` is the name of the nonlinear solver (see Chapter 12 for details).

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

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

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

    Call the appropriate set functions for the selected nonlinear solver module to change optional inputs specific to that nonlinear solver. These *must* be called after `IDAInit` if using the default nonlinear solver or after attaching a new nonlinear solver to IDAS, otherwise the optional inputs will be overridden by IDAS defaults. See Chapter 12 for more information on optional inputs.

15. **Correct initial values**

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

16. **Specify rootfinding problem**

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

17. **Advance solution in time**

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

18. **Get optional outputs**

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

19. **Deallocate memory for solution vectors**

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

    `N_VDestroy(yret);`

    and similarly for `ypret`.

20. **Free solver memory**

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

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

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

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

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

23. **Finalize MPI, if used**

    Call `MPI_Finalize()` to terminate MPI.

SUNDIALS provides some linear solvers only as a means for users to get problems running and not as highly efficient solvers. For example, if solving a dense system, we suggest using the LAPACK solvers if the size of the linear system is $> 50,000$. (Thanks to A. Nicolai for his testing and recommendation.) Table 4.1 shows the linear solver interfaces available as SUNLINSOL modules and the vector implementations required for use. As an example, one cannot use the dense direct solver interfaces with the MPI-based vector implementation. However, as discussed in Chapter 11 the SUNDIALS packages operate on generic SUNLINSOL objects, allowing a user to develop their own solvers should they so desire.

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

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

4.5   User-callable functions

This section describes the IDAS functions that are called by the user to set up and solve a DAE. Some of these are required. However, starting with §4.5.8, the functions listed involve optional inputs/outputs or restarting, and those paragraphs can be skipped for a casual use of IDAS. In any case, refer to §4.4 for the correct order of these calls.

On an error, each user-callable function returns a negative value and sends an error message to the error handler routine, which prints the message on `stderr` by default. However, the user can set a file as error output or can provide his own error handler function (see §4.5.8.1).

4.5.1   IDAS initialization and deallocation functions

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

| IDACreate |

Call	`ida_mem = IDACreate();`
Description	The function `IDACreate` instantiates an IDAS solver object.
Arguments	`IDACreate` has no arguments.
Return value	If successful, `IDACreate` returns a pointer to the newly created IDAS memory block (of type `void *`). Otherwise it returns `NULL`.
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 IDAS.	
Arguments	`ida_mem`	(`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`res`	(`IDAResFn`) is the C function which computes the residual function F in the DAE. This function has the form `res(t, yy, yp, resval, user_data)`. For full details see §4.6.1.
	`t0`	(`realtype`) is the initial value of t.
	`y0`	(`N_Vector`) is the initial value of y.
	`yp0`	(`N_Vector`) is the initial value of $\dot{y}$.
Return value	The return value `flag` (of type `int`) will be one of the following:	
	`IDA_SUCCESS`	The call to `IDAInit` was successful.
	`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
	`IDA_MEM_FAIL`	A memory allocation request has failed.
	`IDA_ILL_INPUT`	An input argument to `IDAInit` has an illegal value.
Notes	If an error occurred, `IDAInit` also sends an error message to the error handler function.	
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 IDAS memory block (of type `void *`).
Return value	The function `IDAFree` has no return value.
F2003 Name	`FIDAFree`

4.5.2 IDAS tolerance specification functions

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

IDASStolerances

Call	`flag = IDASStolerances(ida_mem, reltol, abstol);`
Description	The function `IDASStolerances` specifies scalar relative and absolute tolerances.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`reltol` (`realtype`) is the scalar relative error tolerance.
	`abstol` (`realtype`) is the scalar absolute error tolerance.
Return value	The return value `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASStolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_MALLOC`	The allocation function `IDAInit` has not been called.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

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 IDAS memory block returned by `IDACreate`.
	`reltol` (`realtype`) is the scalar relative error tolerance.
	`abstol` (`N_Vector`) is the vector of absolute error tolerances.
Return value	The return value `flag` (of type `int`) will be one of the following:

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

Notes	This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the state vector y.
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. (2.7).
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`efun` (`IDAEwtFn`) is the C function which defines the `ewt` vector (see §4.6.3).
Return value	The return value `flag` (of type `int`) will be one of the following:

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

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 `idasRoberts_dns` in the IDAS package, and the discussion of it in the IDAS Examples document [54]. In that problem, the three components vary between 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

(3) Finally, it is important to pick all the tolerance values conservatively, because they control the error committed on each individual time step. The final (global) errors are a sort of accumulation of those per-step errors. A good rule of thumb is to reduce the tolerances by a factor of .01 from the actual desired limits on errors. So if you want .01% accuracy (globally), a good choice is `reltol`$= 10^{-6}$. But in any case, it is a good idea to do a few experiments with the tolerances to see how the computed solution values vary as tolerances are reduced.

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

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

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

(3) The user's residual routine `res` should never change a negative value in the solution vector `yy` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `res` routine

cannot tolerate a zero or negative value (e.g., because there is a square root or log of it), then the offending value should be changed to zero or a tiny positive number in a temporary variable (not in the input yy vector) for the purposes of computing $F(t, y, \dot{y})$.

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

4.5.3 Linear solver interface functions

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

With most iterative linear solvers, preconditioning can be done on the left only, on the right only, on both the left and the right, or not at all. The exceptions to this rule are SPFGMR that supports right preconditioning only and PCG that performs symmetric preconditioning. However, in IDAS only left preconditioning is supported. For the specification of a preconditioner, see the iterative linear solver sections in §4.5.8 and §4.6. A preconditioner matrix P must approximate the Jacobian J, at least crudely.

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

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

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

Alternately, a user-supplied `SUNLinearSolver` module may be created and used instead. The use of each of the generic linear solvers involves certain constants, functions and possibly some macros, that are likely to be needed in the user code. These are available in the corresponding header file associated with the specific SUNMATRIX or SUNLINSOL module in question, as described in Chapters 10 and 11.

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

`IDASetLinearSolver`

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

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

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

            `LS`   (`SUNLinearSolver`) SUNLINSOL object to use for solving linear systems of the form (2.5.

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

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

IDALS_SUCCESS   The IDALS initialization was successful.

IDALS_MEM_NULL   The ida_mem pointer is NULL.

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

IDALS_SUNLS_FAIL A call to the LS object failed.

IDALS_MEM_FAIL   A memory allocation request failed.

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

             The previous routines IDADlsSetLinearSolver and IDASpilsSetLinearSolver are
             now wrappers for this routine, and may still be used for backward-compatibility. How-
             ever, 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 IDAS uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNON-
LINSOL_NEWTON module (see §12.3). To specify a different nonlinear solver in IDAS, the user's program
must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must
then attach the SUNNONLINSOL object to IDAS by calling IDASetNonlinearSolver, as documented
below.

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

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

| IDASetNonlinearSolver |

Call   flag = IDASetNonlinearSolver(ida_mem, NLS);

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

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

             NLS   (SUNNonlinearSolver) SUNNONLINSOL object to use for solving nonlinear sys-
                     tems.

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

IDA_SUCCESS   The nonlinear solver was successfully attached.

IDA_MEM_NULL   The ida_mem pointer is NULL.

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

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

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 IDAS memory block.

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

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

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

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

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

IDA_SUCCESS	IDASolve succeeded.
IDA_MEM_NULL	The argument ida_mem was NULL.
IDA_NO_MALLOC	The allocation function IDAInit has not been called.
IDA_ILL_INPUT	One of the input arguments was illegal.
IDA_LSETUP_FAIL	The linear solver's setup function failed in an unrecoverable manner.
IDA_LINIT_FAIL	The linear solver's initialization function failed.
IDA_LSOLVE_FAIL	The linear solver's solve function failed in an unrecoverable manner.
IDA_BAD_EWT	Some component of the error weight vector is zero (illegal), either for the input value of y0 or a corrected value.
IDA_FIRST_RES_FAIL	The user's residual function returned a recoverable error flag on the first call, but IDACalcIC was unable to recover.
IDA_RES_FAIL	The user's residual function returned a nonrecoverable error flag.
IDA_NO_RECOVERY	The user's residual function, or the linear solver's setup or solve function had a recoverable error, but IDACalcIC was unable to recover.
IDA_CONSTR_FAIL	IDACalcIC was unable to find a solution satisfying the inequality constraints.

IDA_LINESEARCH_FAIL	The linesearch algorithm failed to find a solution with a step larger than `steptol` in weighted RMS norm, and within the allowed number of backtracks.
IDA_CONV_FAIL	IDACalcIC failed to get convergence of the Newton iterations.

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

Note that IDACalcIC will correct the values of $y(t_0)$ and $\dot{y}(t_0)$ which were specified in the previous call to IDAInit or IDAReInit. To obtain the corrected values, call IDAGetconsistentIC (see §4.5.10.3).

F2003 Name   `FIDACalcIC`

4.5.6   Rootfinding initialization function

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

IDARootInit

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

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

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

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

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

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

           IDA_SUCCESS   The call to IDARootInit was successful.

           IDA_MEM_NULL   The `ida_mem` argument was NULL.

           IDA_MEM_FAIL   A memory allocation failed.

           IDA_ILL_INPUT   The function g is NULL, but `nrtfn> 0`.

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

F2003 Name   `FIDARootInit`

4.5.7   IDAS solver function

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

IDASolve

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

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

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

           `tout`   (`realtype`) the next time at which a computed solution is desired.

           `tret`   (`realtype`) the time reached by the solver (output).

yret   (N_Vector) the computed solution vector y.

ypret   (N_Vector) the computed solution vector $\dot{y}$.

itask   (int) a flag indicating the job of the solver for the next user step. The IDA_NORMAL task is to have the solver take internal steps until it has reached or just passed the user specified tout parameter. The solver then interpolates in order to return approximate values of $y(\texttt{tout})$ and $\dot{y}(\texttt{tout})$. The IDA_ONE_STEP option tells the solver to just take one internal step and return the solution at the point reached by that step.

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

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

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

IDA_SUCCESS	IDASolve succeeded.
IDA_TSTOP_RETURN	IDASolve succeeded by reaching the stop point specified through the optional input function IDASetStopTime. See §4.5.8.1 for more information.
IDA_ROOT_RETURN	IDASolve succeeded and found one or more roots. In this case, tret is the location of the root. If $\texttt{nrtfn} > 1$, 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 IDAS solver. IDAS provides functions that can be used to change these optional input parameters from their default values. Table 4.2 lists all optional input functions in IDAS which are then described in detail in the remainder of this section. For the most casual use of IDAS, the reader can skip to §4.6.

We note that, on an error return, all 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 IDAS messages should be directed when the default IDAS error handler function is used.

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

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

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

              `IDA_SUCCESS`   The optional value has been successfully set.

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

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

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

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

F2003 Name   `FIDASetErrFile`

Table 4.2: Optional inputs for IDAS and IDALS

Optional input	Function name	Default
IDAS main solver		
Pointer to an error file	IDASetErrFile	stderr
Error handler function	IDASetErrHandlerFn	internal fn.
User data	IDASetUserData	NULL
Maximum order for BDF method	IDASetMaxOrd	5
Maximum no. of internal steps before t_{out}	IDASetMaxNumSteps	500
Initial step size	IDASetInitStep	estimated
Maximum absolute step size	IDASetMaxStep	∞
Value of t_{stop}	IDASetStopTime	∞
Maximum no. of error test failures	IDASetMaxErrTestFails	10
Maximum no. of nonlinear iterations	IDASetMaxNonlinIters	4
Maximum no. of convergence failures	IDASetMaxConvFails	10
Coeff. in the nonlinear convergence test	IDASetNonlinConvCoef	0.33
Suppress alg. vars. from error test	IDASetSuppressAlg	SUNFALSE
Variable types (differential/algebraic)	IDASetId	NULL
Inequality constraints on solution	IDASetConstraints	NULL
Direction of zero-crossing	IDASetRootDirection	both
Disable rootfinding warnings	IDASetNoInactiveRootWarn	none
IDAS initial conditions calculation		
Coeff. in the nonlinear convergence test	IDASetNonlinConvCoefIC	0.0033
Maximum no. of steps	IDASetMaxNumStepsIC	5
Maximum no. of Jacobian/precond. evals.	IDASetMaxNumJacsIC	4
Maximum no. of Newton iterations	IDASetMaxNumItersIC	10
Max. linesearch backtracks per Newton iter.	IDASetMaxBacksIC	100
Turn off linesearch	IDASetLineSearchOffIC	SUNFALSE
Lower bound on Newton step	IDASetStepToleranceIC	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

IDASetErrHandlerFn

Call	`flag = IDASetErrHandlerFn(ida_mem, ehfun, eh_data);`
Description	The function `IDASetErrHandlerFn` specifies the optional user-defined function to be used in handling error messages.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`ehfun` (`IDAErrHandlerFn`) is the user's C error handler function (see §4.6.2).
	`eh_data` (`void *`) pointer to user data passed to `ehfun` every time it is called.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The function `ehfun` and data pointer `eh_data` have been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
Notes	Error messages indicating that the IDAS solver memory is `NULL` will always be directed to `stderr`.
F2003 Name	`FIDASetErrHandlerFn`

IDASetUserData

Call	`flag = IDASetUserData(ida_mem, user_data);`
Description	The function `IDASetUserData` specifies the user data block `user_data` and attaches it to the main IDAS memory block.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`user_data` (`void *`) pointer to the user data.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
Notes	If specified, the pointer to `user_data` is passed to all user-supplied functions that have it as an argument. Otherwise, a `NULL` pointer is passed.
	If `user_data` is needed in user linear solver or preconditioner functions, the call to `IDASetUserData` must be made *before* the call to specify the linear solver.
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 IDAS memory block.
	`maxord` (`int`) value of the maximum method order. This must be positive.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
	`IDA_ILL_INPUT` The input value `maxord` is ≤ 0, or larger than its previous value.
Notes	The default value is 5. If the input value exceeds 5, the value 5 will be used. Since `maxord` affects the memory requirements for the internal IDAS memory block, its value cannot be increased past its previous value.
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 IDAS memory block.

                `mxsteps` (`long int`) maximum allowed number of steps.

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

                IDA_SUCCESS   The optional value has been successfully set.

                IDA_MEM_NULL   The `ida_mem` pointer is `NULL`.

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

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

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 IDAS memory block.

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

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

                IDA_SUCCESS   The optional value has been successfully set.

                IDA_MEM_NULL The `ida_mem` pointer is `NULL`.

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

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 IDAS memory block.

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

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

                IDA_SUCCESS   The optional value has been successfully set.

                IDA_MEM_NULL   The `ida_mem` pointer is `NULL`.

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

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

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 IDAS memory block.
	`tstop` (`realtype`) value of the independent variable past which the solution should not proceed.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
	`IDA_ILL_INPUT` The value of `tstop` is not beyond the current t value, t_n.
Notes	The default, if this routine is not called, is that no stop time is imposed.
	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 IDAS memory block.
	`maxnef` (`int`) maximum number of error test failures allowed on one step (> 0).
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
Notes	The default value is 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 IDAS memory block.
	`maxcor` (`int`) maximum number of nonlinear solver iterations allowed on one step (> 0).
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
	`IDA_MEM_FAIL` The SUNNONLINSOL module is `NULL`.
Notes	The default value is 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 IDAS memory block.
	`maxncf` (`int`) maximum number of allowable nonlinear solver convergence failures on one step (> 0).
Return value	The return value `flag` (of type `int`) is one of
	IDA_SUCCESS The optional value has been successfully set.
	IDA_MEM_NULL The `ida_mem` pointer is NULL.
Notes	The default value is 10.
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. (2.8).
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`nlscoef` (`realtype`) coefficient in nonlinear convergence test (> 0.0).
Return value	The return value `flag` (of type `int`) is one of
	IDA_SUCCESS The optional value has been successfully set.
	IDA_MEM_NULL The `ida_mem` pointer is NULL.
	IDA_ILL_INPUT The value of `nlscoef` is $<= 0.0$.
Notes	The default value is 0.33.
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 IDAS memory block.
	`suppressalg` (`booleantype`) indicates whether to suppress (`SUNTRUE`) or not (`SUNFALSE`) the algebraic variables in the local error test.
Return value	The return value `flag` (of type `int`) is one of
	IDA_SUCCESS The optional value has been successfully set.
	IDA_MEM_NULL The `ida_mem` pointer is NULL.
Notes	The default value is `SUNFALSE`.
	If `suppressalg=SUNTRUE` is selected, then the `id` vector must be set (through `IDASetId`) to specify the algebraic components.
	In general, the use of this option (with `suppressalg = SUNTRUE`) is *discouraged* when solving DAE systems of index 1, whereas it is generally *encouraged* for systems of index 2 or more. See pp. 146-147 of Ref. [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 IDAS memory block.
	`id` (`N_Vector`) state vector. A value of 1.0 indicates a differential variable, while 0.0 indicates an algebraic variable.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
Notes	The vector `id` is required if the algebraic variables are to be suppressed from the local error test (see `IDASetSuppressAlg`) or if `IDACalcIC` is to be called with `icopt` = `IDA_YA_YDP_INIT` (see §4.5.5).
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 IDAS memory block.
	`constraints` (`N_Vector`) vector of constraint flags. If `constraints[i]` is
	$\quad$ 0.0 then no constraint is imposed on y_i.
	$\quad$ 1.0 then y_i will be constrained to be $y_i \geq 0.0$.
	$\quad$ −1.0 then y_i will be constrained to be $y_i \leq 0.0$.
	$\quad$ 2.0 then y_i will be constrained to be $y_i > 0.0$.
	$\quad$ −2.0 then y_i will be constrained to be $y_i < 0.0$.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
	`IDA_ILL_INPUT` The constraints vector contains illegal values or the simultaneous corrector option has been selected when doing forward sensitivity analysis.
Notes	The presence of a non-`NULL` constraints vector that is not 0.0 in all components will cause constraint checking to be performed. However, a call with 0.0 in all components of `constraints` will result in an illegal input return.
	Constraint checking when doing forward sensitivity analysis with the simultaneous corrector option is currently disallowed and will result in an illegal input return.
F2003 Name	`FIDASetConstraints`

4.5.8.2 Linear solver interface optional input functions

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

When using matrix-based linear solver modules, the IDALS solver interface needs a function to compute an approximation to the Jacobian matrix $J(t, y, \dot{y})$. This function must be of type `IDALsJacFn`.

The user can supply a Jacobian function, or if using a dense or banded matrix J can use the default internal difference quotient approximation that comes with the IDALS interface. To specify a user-supplied Jacobian function `jac`, IDALS provides the function `IDASetJacFn`. The IDALS interface passes the pointer `user_data` to the Jacobian function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer `user_data` may be specified through `IDASetUserData`.

`IDASetJacFn`

Call	`flag = IDASetJacFn(ida_mem, jac);`
Description	The function `IDASetJacFn` specifies the Jacobian approximation function to be used for a matrix-based solver within the IDALS interface.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`jac` (`IDALsJacFn`) user-defined Jacobian approximation function.
Return value	The return value `flag` (of type `int`) is one of
	IDALS_SUCCESS The optional value has been successfully set.
	IDALS_MEM_NULL The `ida_mem` pointer is `NULL`.
	IDALS_LMEM_NULL The IDALS linear solver interface has not been initialized.
Notes	This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.
	By default, IDALS uses an internal difference quotient function for dense and band matrices. If `NULL` is passed to `jac`, this default function is used. An error will occur if no `jac` is supplied when using other matrix types.
	The function type `IDALsJacFn` is described in §4.6.5.
	The previous routine `IDADlsSetJacFn` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.
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 §11.4.1 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 §11.4.1.
Arguments	`ida_mem` (`void *`) pointer to the IDAS 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 IDAS memory block.

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

              `jtimes`   (`IDALsJacTimesVecFn`) user-defined Jacobian-vector product function.

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

              `IDALS_SUCCESS`   The optional value has been successfully set.

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

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

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

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

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

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

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

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

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 IDAS memory block.

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

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

            IDALS_SUCCESS   The optional value has been successfully set.

            IDALS_MEM_NULL   The ida_mem pointer is NULL.

            IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

            IDALS_ILL_INPUT The specified value of dqincfac is ≤ 0.

Notes   The default value is 1.0.

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

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

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 [28] 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 IDAS 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 IDAS 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

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

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

`IDASetPreconditioner`

Call	`flag = IDASetPreconditioner(ida_mem, psetup, psolve);`
Description	The function `IDASetPreconditioner` specifies the preconditioner setup and solve functions.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`psetup` (`IDALsPrecSetupFn`) user-defined function to set up the preconditioner. Pass `NULL` if no setup is necessary.
	`psolve` (`IDALsPrecSolveFn`) user-defined preconditioner solve function.
Return value	The return value `flag` (of type `int`) is one of
	`IDALS_SUCCESS` The optional values have been successfully set.
	`IDALS_MEM_NULL` The `ida_mem` pointer is `NULL`.
	`IDALS_LMEM_NULL` The IDALS linear solver has not been initialized.
	`IDALS_SUNLS_FAIL` An error occurred when setting up preconditioning in the SUNLINSOL object used by the IDALS interface.
Notes	The default is `NULL` for both arguments (i.e., no preconditioning).
	This function must be called *after* the IDALS linear solver interface has been initialized through a call to `IDASetLinearSolver`.
	The function type `IDALsPrecSolveFn` is described in §4.6.8.
	The function type `IDALsPrecSetupFn` is described in §4.6.9.
	The previous routine `IDASpilsSetPreconditioner` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.
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 IDAS memory block.

eplifac (`realtype`) linear convergence safety factor (≥ 0.0).

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

IDALS_SUCCESS   The optional value has been successfully set.

IDALS_MEM_NULL   The `ida_mem` pointer is `NULL`.

IDALS_LMEM_NULL   The IDALS linear solver has not been initialized.

IDALS_ILL_INPUT   The factor `eplifac` is negative.

Notes   The default value is 0.05.

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

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

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

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 IDAS 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 (IDAS v4.0.0) 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 IDAS memory block.

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

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

IDA_SUCCESS   The optional value has been successfully set.

IDA_MEM_NULL   The `ida_mem` pointer is `NULL`.

IDA_ILL_INPUT The `epiccon` factor is $<= 0.0$.

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

This test uses a weighted RMS norm (with weights defined by the tolerances). For new initial value vectors y and $\dot{y}$ to be accepted, the norm of $J^{-1}F(t_0, y, \dot{y})$ must be $\le$ 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 IDAS memory block.

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

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

IDA_SUCCESS   The optional value has been successfully set.

IDA_MEM_NULL   The `ida_mem` pointer is `NULL`.

IDA_ILL_INPUT `maxnh` is non-positive.

Notes   The default value is 5.

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 IDAS memory block.

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

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

IDA_SUCCESS   The optional value has been successfully set.

IDA_MEM_NULL   The `ida_mem` pointer is `NULL`.

IDA_ILL_INPUT `maxnj` is non-positive.

Notes   The default value is 4.

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 IDAS memory block.

maxnit (int) maximum number of Newton iterations.

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

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

IDA_ILL_INPUT maxnit is non-positive.

Notes The default value is 10.

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 IDAS memory block.

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

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

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

IDA_ILL_INPUT maxbacks is non-positive.

Notes The default value is 100.

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

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 IDAS memory block.

lsoff (booleantype) a flag to turn off (SUNTRUE) or keep (SUNFALSE) the linesearch algorithm.

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

IDA_SUCCESS The optional value has been successfully set.

IDA_MEM_NULL The ida_mem pointer is NULL.

Notes The default value is SUNFALSE.

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 IDAS memory block.

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

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

IDA_SUCCESS   The optional value has been successfully set.

IDA_MEM_NULL   The ida_mem pointer is NULL.

IDA_ILL_INPUT   The steptol tolerance is $<= 0.0$.

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

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 IDAS memory block.

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

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

              IDA_SUCCESS   The optional value has been successfully set.

              IDA_MEM_NULL   The ida_mem pointer is NULL.

              IDA_ILL_INPUT   rootfinding has not been activated through a call to IDARootInit.

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

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 IDAS memory block.

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

              IDA_SUCCESS   The optional value has been successfully set.

              IDA_MEM_NULL   The ida_mem pointer is NULL.

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

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 IDAS.

The call to the IDAGetDky function has the following form:

IDAGetDky

Call	`flag = IDAGetDky(ida_mem, t, k, dky);`
Description	The function `IDAGetDky` computes the interpolated values of the kth derivative of y for any value of t in the last internal step taken by IDAS. The value of k must be non-negative and smaller than the last internal order used. A value of 0 for k means that the y is interpolated. The value of t must satisfy $t_n - h_u \leq t \leq t_n$, where t_n denotes the current internal time reached, and h_u is the last internal step size used successfully.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`t` (`realtype`) time at which to interpolate.
	`k` (`int`) integer specifying the order of the derivative of y wanted.
	`dky` (`N_Vector`) vector containing the interpolated k^{th} derivative of $y(t)$.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` `IDAGetDky` succeeded.
	`IDA_MEM_NULL` The `ida_mem` argument was `NULL`.
	`IDA_BAD_T` `t` is not in the interval $[t_n - h_u, t_n]$.
	`IDA_BAD_K` `k` is not one of $\{0, 1, \ldots, klast\}$.
	`IDA_BAD_DKY` `dky` is `NULL`.
Notes	It is only legal to call the function `IDAGetDky` after a successful return from `IDASolve`. Functions `IDAGetCurrentTime`, `IDAGetLastStep` and `IDAGetLastOrder` (see §4.5.10.2) can be used to access t_n, h_u and $klast$.
F2003 Name	`FIDAGetDky`

4.5.10 Optional output functions

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

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

4.5.10.1 SUNDIALS version information

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

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.

Table 4.3: Optional outputs from IDAS and IDALS

Optional output	Function name
IDAS main solver	
Size of IDAS real and integer workspace	`IDAGetWorkSpace`
Cumulative number of internal steps	`IDAGetNumSteps`
No. of calls to residual function	`IDAGetNumResEvals`
No. of calls to linear solver setup function	`IDAGetNumLinSolvSetups`
No. of local error test failures that have occurred	`IDAGetNumErrTestFails`
Order used during the last step	`IDAGetLastOrder`
Order to be attempted on the next step	`IDAGetCurrentOrder`
Order reductions due to stability limit detection	`IDAGetNumStabLimOrderReds`
Actual initial step size used	`IDAGetActualInitStep`
Step size used for the last step	`IDAGetLastStep`
Step size to be attempted on the next step	`IDAGetCurrentStep`
Current internal time reached by the solver	`IDAGetCurrentTime`
Suggested factor for tolerance scaling	`IDAGetTolScaleFactor`
Error weight vector for state variables	`IDAGetErrWeights`
Estimated local errors	`IDAGetEstLocalErrors`
No. of nonlinear solver iterations	`IDAGetNumNonlinSolvIters`
No. of nonlinear convergence failures	`IDAGetNumNonlinSolvConvFails`
Array showing roots found	`IDAGetRootInfo`
No. of calls to user root function	`IDAGetNumGEvals`
Name of constant associated with a return flag	`IDAGetReturnFlagName`
IDAS initial conditions calculation	
Number of backtrack operations	`IDAGetNumBacktrackOps`
Corrected initial conditions	`IDAGetConsistentIC`
IDALS linear solver interface	
Size of real and integer workspace	`IDAGetLinWorkSpace`
No. of Jacobian evaluations	`IDAGetNumJacEvals`
No. of residual calls for finite diff. Jacobian[-vector] evals.	`IDAGetNumLinResEvals`
No. of linear iterations	`IDAGetNumLinIters`
No. of linear convergence failures	`IDAGetNumLinConvFails`
No. of preconditioner evaluations	`IDAGetNumPrecEvals`
No. of preconditioner solves	`IDAGetNumPrecSolves`
No. of Jacobian-vector setup evaluations	`IDAGetNumJTSetupEvals`
No. of Jacobian-vector product evaluations	`IDAGetNumJtimesEvals`
Last return from a linear solver function	`IDAGetLastLinFlag`
Name of constant associated with a return flag	`IDAGetLinReturnFlagName`

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

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

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

SUNDIALSGetVersionNumber

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

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

Arguments   major (int) SUNDIALS release major version number.
            minor (int) SUNDIALS release minor version number.
            patch (int) SUNDIALS release patch version number.
            label (char *) character array to hold the SUNDIALS release label.
            len   (int) allocated length of the label character array.

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

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

4.5.10.2   Main solver optional output functions

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

IDAGetWorkSpace

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

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

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

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

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

Notes   In terms of the problem size N, the maximum method order maxord, and the number nrtfn of root functions (see §4.5.6), the actual size of the real workspace, in realtype words, is given by the following:

            • base value: lenrw $= 55 + (m + 6) * N_r + 3*$nrtfn;
            • with IDASVtolerances: lenrw $=$ lenrw $+N_r$;

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

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

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

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

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

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

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

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 IDAS memory block.
              nsteps (long int) number of steps taken by IDAS.

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

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

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 IDAS memory block.
              nrevals (long int) number of calls to the user's res function.

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

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

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

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 IDAS memory block.

             `nlinsetups` (`long int`) number of calls made to the linear solver setup function.

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

             IDA_SUCCESS   The optional output value has been successfully set.

             IDA_MEM_NULL The `ida_mem` pointer is NULL.

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 IDAS memory block.

             `netfails` (`long int`) number of error test failures.

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

             IDA_SUCCESS   The optional output value has been successfully set.

             IDA_MEM_NULL The `ida_mem` pointer is NULL.

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 IDAS memory block.

             `klast`   (`int`) method order used on the last internal step.

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

             IDA_SUCCESS   The optional output value has been successfully set.

             IDA_MEM_NULL The `ida_mem` pointer is NULL.

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 IDAS memory block.

             `kcur`   (`int`) method order to be used on the next internal step.

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

             IDA_SUCCESS   The optional output value has been successfully set.

             IDA_MEM_NULL The `ida_mem` pointer is NULL.

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 IDAS memory block.
	`hlast` (`realtype`) step size taken on the last internal step by IDAS, or last artificial step size used in `IDACalcIC`, whichever was called last.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional output value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is NULL.
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 IDAS memory block.
	`hcur` (`realtype`) step size to be attempted on the next internal step.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional output value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is NULL.
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 IDAS memory block.
	`hinused` (`realtype`) actual value of initial step size.
Return value	The return value `flag` (of type `int`) is one of
	`IDA_SUCCESS` The optional output value has been successfully set.
	`IDA_MEM_NULL` The `ida_mem` pointer is NULL.
Notes	Even if the value of the initial integration step size was specified by the user through a call to `IDASetInitStep`, this value might have been changed by IDAS to ensure that the step size is within the prescribed bounds ($h_{\min} \leq h_0 \leq h_{\max}$), 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 IDAS memory block.
	`tcur` (`realtype`) current internal time reached.

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

         IDA_SUCCESS   The optional output value has been successfully set.

         IDA_MEM_NULL The `ida_mem` pointer is `NULL`.

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 IDAS memory block.

         `tolsfac` (`realtype`) suggested scaling factor for user tolerances.

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

         IDA_SUCCESS   The optional output value has been successfully set.

         IDA_MEM_NULL The `ida_mem` pointer is `NULL`.

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. (2.7) (or by the user's `IDAEwtFn`).

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

         `eweight` (`N_Vector`) solution error weights at the current time.

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

         IDA_SUCCESS   The optional output value has been successfully set.

         IDA_MEM_NULL The `ida_mem` pointer is `NULL`.

Notes   The user must allocate space for `eweight`.

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 IDAS memory block.

         `ele`   (`N_Vector`) estimated local errors at the current time.

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

         IDA_SUCCESS   The optional output value has been successfully set.

         IDA_MEM_NULL The `ida_mem` pointer is `NULL`.

Notes   The user must allocate space for `ele`.

               The values returned in `ele` are only valid if `IDASolve` returned a non-negative value.

               The `ele` vector, togther with the `eweight` vector from `IDAGetErrWeights`, can be used to determine how the various components of the system contributed to the estimated local error test. Specifically, that error test uses the RMS norm of a vector whose components are the products of the components of these two vectors. Thus, for example, if there were recent error test failures, the components causing the failures are those with largest values for the products, denoted loosely as `eweight[i]*ele[i]`.

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 IDAS integrator statistics as a group.

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

`nsteps`   (`long int`) cumulative number of steps taken by IDAS.

`nrevals`   (`long int`) cumulative number of calls to the user's `res` function.

`nlinsetups` (`long int`) cumulative number of calls made to the linear solver setup function.

`netfails`   (`long int`) cumulative number of error test failures.

`klast`   (`int`) method order used on the last internal step.

`kcur`   (`int`) method order to be used on the next internal step.

`hinused`   (`realtype`) actual value of initial step size.

`hlast`   (`realtype`) step size taken on the last internal step.

`hcur`   (`realtype`) step size to be attempted on the next internal step.

`tcur`   (`realtype`) current internal time reached.

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

IDA_SUCCESS   the optional output values have been successfully set.

IDA_MEM_NULL the `ida_mem` pointer is NULL.

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 IDAS memory block.

`nniters` (`long int`) number of nonlinear iterations performed.

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

IDA_SUCCESS   The optional output value has been successfully set.

IDA_MEM_NULL The `ida_mem` pointer is NULL.

IDA_MEM_FAIL The SUNNONLINSOL module is NULL.

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 IDAS memory block.

`nncfails` (`long int`) number of nonlinear convergence failures.

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

IDA_SUCCESS   The optional output value has been successfully set.

IDA_MEM_NULL The `ida_mem` pointer is NULL.

F2003 Name `FIDAGetNumNonlinSolvConvFails`

IDAGetNonlinSolvStats

Call   `flag = IDAGetNonlinSolvStats(ida_mem, &nniters, &nncfails);`

Description   The function `IDAGetNonlinSolvStats` returns the IDAS nonlinear solver statistics as a group.

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

               `nniters`   (`long int`) cumulative number of nonlinear iterations performed.

               `nncfails` (`long int`) cumulative number of nonlinear convergence failures.

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

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

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

               `IDA_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

F2003 Name   `FIDAGetNonlinSolvStats`

IDAGetReturnFlagName

Call   `name = IDAGetReturnFlagName(flag);`

Description   The function `IDAGetReturnFlagName` returns the name of the IDAS constant corresponding to `flag`.

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

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

F2003 Name   `FIDAGetReturnFlagName`

4.5.10.3   Initial condition calculation optional output functions

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IDAGetNumBcktrackOps

Call   `flag = IDAGetNumBacktrackOps(ida_mem, &nbacktr);`

Description   The function `IDAGetNumBacktrackOps` returns the number of backtrack operations done in the linesearch algorithm in `IDACalcIC`.

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

               `nbacktr` (`long int`) the cumulative number of backtrack operations.

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

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

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

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 IDAS memory block.

               `yy0_mod` (`N_Vector`) consistent solution vector.

               `yp0_mod` (`N_Vector`) consistent derivative vector.

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

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

IDA_ILL_INPUT The function was not called before the first call to IDASolve.

IDA_MEM_NULL The ida_mem pointer is NULL.

Notes   If the consistent solution vector or consistent derivative vector is not desired, pass NULL
                  for the corresponding argument.

                  The user must allocate space for yy0_mod and yp0_mod (if not NULL).

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 IDAS memory block.

                  rootsfound (int *) array of length nrtfn with the indices of the user functions g_i
                       found to have a root. For $i = 0, \ldots,$ nrtfn -1, rootsfound[i] $\neq 0$ if g_i has a
                       root, and $= 0$ if not.

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

                  IDA_SUCCESS   The optional output values have been successfully set.

                  IDA_MEM_NULL The ida_mem pointer is NULL.

Notes   Note that, for the components g_i for which a root was found, the sign of rootsfound[i]
                  indicates the direction of zero-crossing. A value of $+1$ indicates that g_i is increasing,
                  while a value of -1 indicates a decreasing g_i.

                  The user must allocate memory for the vector rootsfound.

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 IDAS memory block.

                  ngevals (long int) number of calls to the user's function g so far.

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

                  IDA_SUCCESS   The optional output value has been successfully set.

                  IDA_MEM_NULL The ida_mem pointer is NULL.

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 IDAS memory block.

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

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

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

                 IDALS_SUCCESS   The optional output value has been successfully set.

                 IDALS_MEM_NULL   The `ida_mem` pointer is NULL.

                 IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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

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 IDAS memory block.

                      `njevals` (`long int`) the cumulative number of calls to the Jacobian function (total so far).

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

                 IDALS_SUCCESS   The optional output value has been successfully set.

                 IDALS_MEM_NULL   The `ida_mem` pointer is NULL.

                 IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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 IDAS memory block.

                      `nrevalsLS` (`long int`) the cumulative number of calls to the user residual function.

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

IDALS_SUCCESS   The optional output value has been successfully set.

IDALS_MEM_NULL   The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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

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 IDAS memory block.

nliters (long int) the current number of linear iterations.

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

IDALS_SUCCESS   The optional output value has been successfully set.

IDALS_MEM_NULL   The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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 IDAS memory block.

nlcfails (long int) the current number of linear convergence failures.

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

IDALS_SUCCESS   The optional output value has been successfully set.

IDALS_MEM_NULL   The ida_mem pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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 IDAS memory block.

npevals (`long int`) the cumulative number of calls to `psetup`.

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

IDALS_SUCCESS   The optional output value has been successfully set.

IDALS_MEM_NULL   The `ida_mem` pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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 IDAS memory block.

              `npsolves` (`long int`) the cumulative number of calls to `psolve`.

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

IDALS_SUCCESS   The optional output value has been successfully set.

IDALS_MEM_NULL   The `ida_mem` pointer is NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

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

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 IDAS memory block.

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

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

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 IDAS memory block.

             `njvevals` (`long int`) the cumulative number of calls to `jtimes`.

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

          `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 IDAS memory block.

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

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

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

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

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

Notes   If the IDALS setup function failed (i.e., `IDASolve` returned `IDA_LSETUP_FAIL`) when using the SUNLINSOL_DENSE or SUNLINSOL_BAND modules, then the value of `lsflag` is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the (dense or banded) Jacobian matrix.

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

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

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

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   IDAS reinitialization function

The function `IDAReInit` reinitializes the main IDAS solver for the solution of a new problem, where a prior call to `IDAInit` has been made. The new problem must have the same size as the previous one. `IDAReInit` performs the same input checking and initializations that `IDAInit` does, but does no memory allocation, as it assumes that the existing internal memory is sufficient for the new problem. A call to `IDAReInit` deletes the solution history that was stored internally during the previous integration. Following a successful call to `IDAReInit`, call `IDASolve` again for the solution of the new problem.

The use of `IDAReInit` requires that the maximum method order, `maxord`, is no larger for the new problem than for the problem specified in the last call to `IDAInit`. In addition, the same NVECTOR module set for the previous problem will be reused for the new problem.

If there are changes to the linear solver specifications, make the appropriate calls to either the linear solver objects themselves, or to the IDALS interface routines, as described in §4.5.3.

If there are changes to any optional inputs, make the appropriate `IDASet***` calls, as described in §4.5.8. Otherwise, all solver inputs set previously remain in effect.

One important use of the `IDAReInit` function is in the treating of jump discontinuities in the residual function. Except in cases of fairly small jumps, it is usually more efficient to stop at each point of discontinuity and restart the integrator with a readjusted DAE model, using a call to `IDAReInit`. To stop when the location of the discontinuity is known, simply make that location a value of tout. To stop when the location of the discontinuity is determined by the solution, use the rootfinding feature. In either case, it is critical that the residual function *not* incorporate the discontinuity, but rather have a smooth extention over the discontinuity, so that the step across it (and subsequent rootfinding, if used) can be done efficiently. Then use a switch within the residual function (communicated through `user_data`) that can be flipped between the stopping of the integration and the restart, so that the restarted problem uses the new values (which have jumped). Similar comments apply if there is to be a jump in the dependent variable vector.

`IDAReInit`

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

Description The function `IDAReInit` provides required problem specifications and reinitializes IDAS.

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

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

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

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

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

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

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

        `IDA_NO_MALLOC` Memory space for the IDAS memory block was not allocated through a previous call to `IDAInit`.

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

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

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, IDAS will attempt to recover (possibly repeating the nonlinear solve, or reducing the step size) in order to avoid this recoverable error return.

             For efficiency reasons, the DAE residual function is not evaluated at the converged solution of the nonlinear solver. Therefore, in general, a recoverable error in that converged value cannot be corrected. (It may be detected when the right-hand side function is called the first time during the following integration step, but a successful step cannot be undone.) However, if the user program also includes quadrature integration, the state variables can be checked for legality in the call to `IDAQuadRhsFn`, which is called at the converged solution of the nonlinear system, and therefore IDAS can be flagged to attempt to recover from such a situation. Also, if sensitivity analysis is performed with the staggered method, the DAE residual function is called at the converged solution of the nonlinear system, and a recoverable error at that point can be flagged, and IDAS will then try to correct it.

             Allocation of memory for `yp` is handled within IDAS.

4.6.2 Error message handler function

As an alternative to the default behavior of directing error and warning messages to the file pointed to by `errfp` (see `IDASetErrFile`), the user may provide a function of type `IDAErrHandlerFn` to process any such messages. The function type `IDAErrHandlerFn` is defined as follows:

IDAErrHandlerFn

Definition	`typedef void (*IDAErrHandlerFn)(int error_code, const char *module,`
	`                                const char *function, char *msg,`
	`                                void *eh_data);`

| Purpose | This function processes error and warning messages from IDAS and its sub-modules. |

Arguments	`error_code` is the error code.
	`module` is the name of the IDAS module reporting the error.
	`function` is the name of the function in which the error occurred.
	`msg` is the error message.
	`eh_data` is a pointer to user data, the same as the `eh_data` parameter passed to `IDASetErrHandlerFn`.

| Return value | A `IDAErrHandlerFn` function has no return value. |

| Notes | `error_code` is negative for errors and positive (`IDA_WARNING`) for warnings. If a function that returns a pointer to memory encounters an error, it sets `error_code` to 0. |

4.6.3 Error weight function

As an alternative to providing the relative and absolute tolerances, the user may provide a function of type `IDAEwtFn` to compute a vector `ewt` containing the multiplicative weights W_i used in the WRMS norm $\| v \|_{\mathrm{WRMS}} = \sqrt{(1/N) \sum_1^N (W_i \cdot v_i)^2}$. These weights will used in place of those defined by Eq. (2.7). The function type `IDAEwtFn` is defined as follows:

IDAEwtFn

| Definition | `typedef int (*IDAEwtFn)(N_Vector y, N_Vector ewt, void *user_data);` |

| Purpose | This function computes the WRMS error weights for the vector y. |

Arguments	`y` is the value of the dependent variable vector at which the weight vector is to be computed.
	`ewt` is the output vector containing the error weights.
	`user_data` is a pointer to user data, the same as the `user_data` parameter passed to `IDASetUserData`.

| Return value | An `IDAEwtFn` function type must return 0 if it successfully set the error weights and -1 otherwise. |

| Notes | Allocation of memory for `ewt` is handled within IDAS. |
| | The error weight vector must have all components positive. It is the user's responsiblity to perform this test and return -1 if it is not satisfied. |

4.6.4 Rootfinding function

If a rootfinding problem is to be solved during the integration of the DAE system, the user must supply a C function of type `IDARootFn`, defined as follows:

IDARootFn

Definition	`typedef int (*IDARootFn)(realtype t, N_Vector y, N_Vector yp,` `                         realtype *gout, void *user_data);`

Purpose   This function computes a vector-valued function $g(t, y, \dot{y})$ such that the roots of the `nrtfn` components $g_i(t, y, \dot{y})$ are to be found during the integration.

Arguments   t   is the current value of the independent variable.

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

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

gout   is the output array, of length `nrtfn`, with components $g_i(t, y, \dot{y})$.

user_data is a pointer to user data, the same as the `user_data` parameter passed to IDASetUserData.

Return value   An `IDARootFn` should return 0 if successful or a non-zero value if an error occurred (in which case the integration is halted and `IDASolve` returns `IDA_RTFUNC_FAIL`).

Notes   Allocation of memory for `gout` is handled within IDAS.

4.6.5   Jacobian construction (matrix-based linear solvers)

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

IDALsJacFn

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

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

Arguments   tt   is the current value of the independent variable t.

cj   is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).

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

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

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

Jac   is the output (approximate) Jacobian matrix (of type `SUNMatrix`), $J = \partial F/\partial y + cj\ \partial F/\partial \dot{y}$.

user_data is a pointer to user data, the same as the `user_data` parameter passed to IDASetUserData.

tmp1

tmp2

tmp3   are pointers to memory allocated for variables of type `N_Vector` which can be used by `IDALsJacFn` function as temporary storage or work space.

Return value   An `IDALsJacFn` should return 0 if successful, a positive value if a recoverable error occurred, or a negative value if a nonrecoverable error occurred.

In the case of a recoverable eror return, the integrator will attempt to recover by reducing the stepsize, and hence changing α in (2.6).

Notes   Information regarding the structure of the specific SUNMATRIX structure (e.g., number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 10 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 §12.1.4 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` = $0 \ldots N - 1$). This macro is meant for small problems for which efficiency of access is not a major concern. Thus, in terms of the indices m and n ranging from 1 to N, the Jacobian element $J_{m,n}$ can be set using the statement `SM_ELEMENT_D(J, m-1, n-1)` = $J_{m,n}$. Alternatively, `SM_COLUMN_D(J, j)` returns a pointer to the first element of the `j`-th column of `Jac` (with `j` = $0 \ldots N - 1$), and the elements of the `j`-th column can then be accessed using ordinary array indexing. Consequently, $J_{m,n}$ can be loaded using the statements `col_n = SM_COLUMN_D(J, n-1)`; `col_n[m-1]` = $J_{m,n}$. For large problems, it is more efficient to use `SM_COLUMN_D` than to use `SM_ELEMENT_D`. Note that both of these macros number rows and columns starting from 0. The SUNMATRIX_DENSE type and accessor macros are documented in §10.3.

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

SUNMATRIX_BAND type and accessor macros are documented in §10.4.

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 §10.5.

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. (2.6).

Arguments
: tt   is the current value of the independent variable.
: yy   is the current value of the dependent variable vector, $y(t)$.
: yp   is the current value of $\dot{y}(t)$.
: rr   is the current value of the residual vector $F(t, y, \dot{y})$.
: v   is the vector by which the Jacobian must be multiplied to the right.
: Jv   is the computed output vector.
: cj   is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).
: user_data is a pointer to user data, the same as the user_data parameter passed to IDASetUserData.
: tmp1
: tmp2   are pointers to memory allocated for variables of type N_Vector which can be used by IDALsJacTimesVecFn as temporary storage or work space.

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

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

: If the user's IDALsJacTimesVecFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to ida_mem to

user_data and then use the IDAGet* functions described in §4.5.10.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

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

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

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

| 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. (2.6)).
user_data	is a pointer to user data, the same as the user_data parameter passed to IDASetUserData.

Return value
The value returned by the Jacobian-vector setup function should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

If the user's IDALsJacTimesVecFn function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to ida_mem to user_data and then use the IDAGet* functions described in §4.5.10.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

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

4.6.8 Preconditioner solve (iterative linear solvers)

If a user-supplied preconditioner is to be used with a SUNLINSOL solver module, then the user must provide a function to solve the linear system $Pz = r$ where P is a left preconditioner matrix which approximates (at least crudely) the Jacobian matrix $J = \partial F / \partial y + cj\ \partial F / \partial \dot{y}$. This function must be of type IDALsPrecSolveFn, defined as follows:

IDALsPrecSolveFn

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

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

Arguments   tt   is the current value of the independent variable.

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

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

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

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

              zvec   is the computed output vector.

              cj   is the scalar in the system Jacobian, proportional to the inverse of the step
                          size (α in Eq. (2.6)).

              delta   is an input tolerance to be used if an iterative method is employed in the
                          solution. In that case, the residual vector $Res = r - Pz$ of the system should
                          be made less than delta in weighted l_2 norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} <$
                          delta. To obtain the N_Vector ewt, call IDAGetErrWeights (see §4.5.10.2).

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

Return value The value to be returned by the preconditioner solve function is a flag indicating whether
              it was successful. This value should be 0 if successful, positive for a recoverable error
              (in which case the step will be retried), negative for an unrecoverable error (in which
              case the integration is halted).

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

4.6.9   Preconditioner setup (iterative linear solvers)

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

IDALsPrecSetupFn

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

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

Arguments   tt   is the current value of the independent variable.

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

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

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

              cj   is the scalar in the system Jacobian, proportional to the inverse of the step
                          size (α in Eq. (2.6)).

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

Return value The value returned by the preconditioner setup function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), negative for an unrecoverable error (in which case the integration is halted).

Notes The operations performed by this function might include forming a crude approximate Jacobian, and performing an LU factorization on the resulting approximation.

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 §12.1.4 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   Integration of pure quadrature equations

IDAS allows the DAE system to include *pure quadratures*. In this case, it is more efficient to treat the quadratures separately by excluding them from the nonlinear solution stage. To do this, begin by excluding the quadrature variables from the vectors `yy` and `yp` and the quadrature equations from within `res`. Thus a separate vector `yQ` of quadrature variables is to satisfy $(d/dt)\mathtt{yQ} = f_Q(t, y, \dot{y})$. The following is an overview of the sequence of calls in a user's main program in this situation. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

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

2. **Set problem dimensions, etc.**

   This generally includes `N`, the problem size N (excluding quadrature variables), `Nq`, the number of quadrature variables, and may include the local vector length `Nlocal` (excluding quadrature variables), and local number of quadrature variables `Nqlocal`.

3. Set vectors of initial values

4. Create IDAS object

5. Initialize IDAS solver

6. Specify integration tolerances

7. Create matrix object

8. Create linear solver object

9. **Set linear solver optional inputs**

10. **Attach linear solver module**

11. **Set optional inputs**

12. **Create nonlinear solver object**

13. **Attach nonlinear solver module**

14. **Set nonlinear solver optional inputs**

15. **Correct initial values**

16. **Set vector of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.

17. **Initialize quadrature integration**

    Call `IDAQuadInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §4.7.1 for details.

18. **Set optional inputs for quadrature integration**

    Call `IDASetQuadErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `IDAQuad*tolerances` functions must be called to specify the integration tolerances for quadrature variables. See §4.7.4 for details.

19. **Advance solution in time**

20. **Extract quadrature variables**

    Call `IDAGetQuad` or `IDAGetQuadDky` to obtain the values of the quadrature variables or their derivatives at the current time. See §4.7.3 for details.

21. **Get optional outputs**

22. **Get quadrature optional outputs**

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

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

24. **Free solver memory**

25. **Free nonlinear solver memory**

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

27. **Finalize MPI, if used**

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

4.7.1 Quadrature initialization and deallocation functions

The function `IDAQuadInit` activates integration of quadrature equations and allocates internal memory related to these calculations. The form of the call to this function is as follows:

IDAQuadInit

Call   `flag = IDAQuadInit(ida_mem, rhsQ, yQ0);`

Description   The function `IDAQuadInit` provides required problem specifications, allocates internal memory, and initializes quadrature integration.

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

               `rhsQ`   (`IDAQuadRhsFn`) is the C function which computes f_Q, the right-hand side of the quadrature equations. This function has the form `fQ(t, yy, yp, rhsQ, user_data)` (for full details see §4.7.6).

               `yQ0`   (`N_Vector`) is the initial value of y_Q.

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

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

               `IDA_MEM_NULL` The IDAS memory was not initialized by a prior call to `IDACreate`.

               `IDA_MEM_FAIL` A memory allocation request failed.

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

F2003 Name   `FIDAQuadInit`

In terms of the number of quadrature variables N_q and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value: `lenrw = lenrw + (maxord+5)`N_q

- If `IDAQuadSVtolerances` is called: `lenrw = lenrw +`N_q

and the size of the integer workspace is increased as follows:

- Base value: `leniw = leniw + (maxord+5)`N_q

- If `IDAQuadSVtolerances` is called: `leniw = leniw +`N_q

    The function `IDAQuadReInit`, useful during the solution of a sequence of problems of same size, reinitializes the quadrature-related internal memory and must follow a call to `IDAQuadInit` (and maybe a call to `IDAReInit`). The number `Nq` of quadratures is assumed to be unchanged from the prior call to `IDAQuadInit`. The call to the `IDAQuadReInit` function has the following form:

IDAQuadReInit

Call   `flag = IDAQuadReInit(ida_mem, yQ0);`

Description   The function `IDAQuadReInit` provides required problem specifications and reinitializes the quadrature integration.

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

               `yQ0`   (`N_Vector`) is the initial value of y_Q.

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

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

               `IDA_MEM_NULL` The IDAS memory was not initialized by a prior call to `IDACreate`.

               `IDA_NO_QUAD`   Memory space for the quadrature integration was not allocated by a prior call to `IDAQuadInit`.

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

F2003 Name   `FIDAQuadReInit`

IDAQuadFree

Call   `IDAQuadFree(ida_mem);`

Description   The function `IDAQuadFree` frees the memory allocated for quadrature integration.

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

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

Notes   In general, `IDAQuadFree` need not be called by the user as it is invoked automatically by `IDAFree`.

F2003 Name   `FIDAQuadFree`

4.7.2   IDAS solver function

Even if quadrature integration was enabled, the call to the main solver function `IDASolve` is exactly the same as in §4.5.7. However, in this case the return value `flag` can also be one of the following:

IDA_QRHS_FAIL   The quadrature right-hand side function failed in an unrecoverable manner.

IDA_FIRST_QRHS_ERR   The quadrature right-hand side function failed at the first call.

IDA_REP_QRHS_ERR   Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. This value will also be returned if the quadrature right-hand side function had repeated recoverable errors during the estimation of an initial step size (assuming the quadrature variables are included in the error tests).

4.7.3   Quadrature extraction functions

If quadrature integration has been initialized by a call to `IDAQuadInit`, or reinitialized by a call to `IDAQuadReInit`, then IDAS computes both a solution and quadratures at time `t`. However, `IDASolve` will still return only the solution y in `y`. Solution quadratures can be obtained using the following function:

IDAGetQuad

Call   `flag = IDAGetQuad(ida_mem, &tret, yQ);`

Description   The function `IDAGetQuad` returns the quadrature solution vector after a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

                 `tret`   (`realtype`) the time reached by the solver (output).

                 `yQ`   (`N_Vector`) the computed quadrature vector.

Return value   The return value `flag` of `IDAGetQuad` is one of:

              `IDA_SUCCESS`   `IDAGetQuad` was successful.

              `IDA_MEM_NULL`   `ida_mem` was NULL.

              `IDA_NO_QUAD`   Quadrature integration was not initialized.

              `IDA_BAD_DKY`   `yQ` is NULL.

F2003 Name   `FIDAGetQuad`

The function `IDAGetQuadDky` computes the `k`-th derivatives of the interpolating polynomials for the quadrature variables at time `t`. This function is called by `IDAGetQuad` with `k = 0` and with the current time at which `IDASolve` has returned, but may also be called directly by the user.

IDAGetQuadDky

Call   `flag = IDAGetQuadDky(ida_mem, t, k, dkyQ);`

Description The function `IDAGetQuadDky` returns derivatives of the quadrature solution vector after a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

       `t`   (`realtype`) the time at which quadrature information is requested. The time `t` must fall within the interval defined by the last successful step taken by IDAS.

       `k`   (`int`) order of the requested derivative. This must be $\leq klast$.

       `dkyQ`   (`N_Vector`) the vector containing the derivative. This vector must be allocated by the user.

Return value The return value `flag` of `IDAGetQuadDky` is one of:

       `IDA_SUCCESS` `IDAGetQuadDky` succeeded.

       `IDA_MEM_NULL` The pointer to `ida_mem` was NULL.

       `IDA_NO_QUAD` Quadrature integration was not initialized.

       `IDA_BAD_DKY` The vector `dkyQ` is `NULL`.

       `IDA_BAD_K`   `k` is not in the range $0, 1, ..., klast$.

       `IDA_BAD_T`   The time `t` is not in the allowed range.

F2003 Name `FIDAGetQuadDky`

4.7.4 Optional inputs for quadrature integration

IDAS provides the following optional input functions to control the integration of quadrature equations.

IDASetQuadErrCon

Call   `flag = IDASetQuadErrCon(ida_mem, errconQ);`

Description The function `IDASetQuadErrCon` specifies whether or not the quadrature variables are to be used in the step size control mechanism within IDAS. If they are, the user must call either `IDAQuadSStolerances` or `IDAQuadSVtolerances` to specify the integration tolerances for the quadrature variables.

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

       `errconQ` (`booleantype`) specifies whether quadrature variables are included (`SUNTRUE`) or not (`SUNFALSE`) in the error control mechanism.

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

       `IDA_SUCCESS` The optional value has been successfully set.

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

       `IDA_NO_QUAD` Quadrature integration has not been initialized.

Notes   By default, `errconQ` is set to `SUNFALSE`.

       It is illegal to call `IDASetQuadErrCon` before a call to `IDAQuadInit`.

F2003 Name `FIDASetQuadErrCon`

If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

IDAQuadSStolerances

Call   flag = IDAQuadSVtolerances(ida_mem, reltolQ, abstolQ);

Description   The function IDAQuadSStolerances specifies scalar relative and absolute tolerances.

Arguments   ida_mem (void *) pointer to the IDAS memory block.
              reltolQ (realtype) is the scalar relative error tolerance.
              abstolQ (realtype) is the scalar absolute error tolerance.

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

              IDA_SUCCESS   The optional value has been successfully set.
              IDA_NO_QUAD   Quadrature integration was not initialized.
              IDA_MEM_NULL   The ida_mem pointer is NULL.
              IDA_ILL_INPUT One of the input tolerances was negative.

F2003 Name   FIDAQuadSStolerances

IDAQuadSVtolerances

Call   flag = IDAQuadSVtolerances(ida_mem, reltolQ, abstolQ);

Description   The function IDAQuadSVtolerances specifies scalar relative and vector absolute toler-
              ances.

Arguments   ida_mem (void *) pointer to the IDAS memory block.
              reltolQ (realtype) is the scalar relative error tolerance.
              abstolQ (N_Vector) is the vector absolute error tolerance.

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

              IDA_SUCCESS   The optional value has been successfully set.
              IDA_NO_QUAD   Quadrature integration was not initialized.
              IDA_MEM_NULL   The ida_mem pointer is NULL.
              IDA_ILL_INPUT One of the input tolerances was negative.

F2003 Name   FIDAQuadSVtolerances

4.7.5   Optional outputs for quadrature integration

IDAS provides the following functions that can be used to obtain solver performance information
related to quadrature integration.

IDAGetQuadNumRhsEvals

Call   flag = IDAGetQuadNumRhsEvals(ida_mem, &nrhsQevals);

Description   The function IDAGetQuadNumRhsEvals returns the number of calls made to the user's
              quadrature right-hand side function.

Arguments   ida_mem (void *) pointer to the IDAS memory block.
              nrhsQevals (long int) number of calls made to the user's rhsQ function.

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

              IDA_SUCCESS   The optional output value has been successfully set.
              IDA_MEM_NULL The ida_mem pointer is NULL.
              IDA_NO_QUAD   Quadrature integration has not been initialized.

F2003 Name   FIDAGetQuadNumRhsEvals

IDAGetQuadNumErrTestFails

Call   `flag = IDAGetQuadNumErrTestFails(ida_mem, &nQetfails);`

Description   The function `IDAGetQuadNumErrTestFails` returns the number of local error test failures due to quadrature variables.

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

                `nQetfails` (`long int`) number of error test failures due to quadrature variables.

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

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

                `IDA_MEM_NULL` The `ida_mem` pointer is NULL.

                `IDA_NO_QUAD`   Quadrature integration has not been initialized.

F2003 Name   `FIDAGetQuadNumErrTestFails`

IDAGetQuadErrWeights

Call   `flag = IDAGetQuadErrWeights(ida_mem, eQweight);`

Description   The function `IDAGetQuadErrWeights` returns the quadrature error weights at the current time.

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

                `eQweight` (`N_Vector`) quadrature error weights at the current time.

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

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

                `IDA_MEM_NULL` The `ida_mem` pointer is NULL.

                `IDA_NO_QUAD`   Quadrature integration has not been initialized.

Notes   The user must allocate memory for `eQweight`.

                If quadratures were not included in the error control mechanism (through a call to `IDASetQuadErrCon` with `errconQ = SUNTRUE`), `IDAGetQuadErrWeights` does not set the `eQweight` vector.

F2003 Name   `FIDAGetQuadErrWeights`

IDAGetQuadStats

Call   `flag = IDAGetQuadStats(ida_mem, &nrhsQevals, &nQetfails);`

Description   The function `IDAGetQuadStats` returns the IDAS integrator statistics as a group.

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

                `nrhsQevals` (`long int`) number of calls to the user's `rhsQ` function.

                `nQetfails` (`long int`) number of error test failures due to quadrature variables.

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

                `IDA_SUCCESS`   the optional output values have been successfully set.

                `IDA_MEM_NULL` the `ida_mem` pointer is NULL.

                `IDA_NO_QUAD`   Quadrature integration has not been initialized.

F2003 Name   `FIDAGetQuadStats`

4.7.6   User-supplied function for quadrature integration

For integration of quadrature equations, the user must provide a function that defines the right-hand side of the quadrature equations (in other words, the integrand function of the integral that must be evaluated). This function must be of type `IDAQuadRhsFn` defined as follows:

IDAQuadRhsFn

Definition	`typedef int (*IDAQuadRhsFn)(realtype t, N_Vector yy, N_Vector yp,` `                            N_Vector rhsQ, void *user_data);`
Purpose	This function computes the quadrature equation right-hand side for a given value of the independent variable t and state vectors y and $\dot{y}$.
Arguments	`t` is the current value of the independent variable.
	`yy` is the current value of the dependent variable vector, $y(t)$.
	`yp` is the current value of the dependent variable derivative vector, $\dot{y}(t)$.
	`rhsQ` is the output vector $f_Q(t, y, \dot{y})$.
	`user_data` is the `user_data` pointer passed to `IDASetUserData`.
Return value	A `IDAQuadRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDA_QRHS_FAIL` is returned).
Notes	Allocation of memory for `rhsQ` is automatically handled within IDAS.
	Both `y` and `rhsQ` are of type `N_Vector`, but they typically have different internal representations. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their `N_Vector` arguments (see §9.3 and §9.4).
	There is one situation in which recovery is not possible even if `IDAQuadRhsFn` function returns a recoverable error flag. This is when this occurs at the very first call to the `IDAQuadRhsFn` (in which case IDAS returns `IDA_FIRST_QRHS_ERR`).

4.8   A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel DAE solver such as IDAS lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (2.5) that must be solved at each time step. The linear algebraic system is large, sparse, and structured. However, if a Krylov iterative method is to be effective in this setting, then a nontrivial preconditioner needs to be used. Otherwise, the rate of convergence of the Krylov iterative method is usually unacceptably slow. Unfortunately, an effective preconditioner tends to be problem-specific.

However, we have developed one type of preconditioner that treats a rather broad class of PDE-based problems. It has been successfully used for several realistic, large-scale problems [41] and is included in a software module within the IDAS package. This module works with the parallel vector module NVECTOR_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix. The blocks need not have the same number of super- and sub-diagonals, and these numbers may vary from block to block. This Band-Block-Diagonal Preconditioner module is called IDABBDPRE.

One way to envision these preconditioners is to think of the domain of the computational PDE problem as being subdivided into M non-overlapping sub-domains. Each of these sub-domains is then assigned to one of the M processors to be used to solve the DAE system. The basic idea is to isolate the preconditioning so that it is local to each processor, and also to use a (possibly cheaper) approximate residual function. This requires the definition of a new function $G(t, y, \dot{y})$ which approximates the function $F(t, y, \dot{y})$ in the definition of the DAE system (2.1). However, the user may set $G = F$. Corresponding to the domain decomposition, there is a decomposition of the solution vectors y and $\dot{y}$ into M disjoint blocks y_m and $\dot{y}_m$, and a decomposition of G into blocks G_m. The block G_m depends on y_m and $\dot{y}_m$, and also on components of $y_{m'}$ and $\dot{y}_{m'}$ associated with neighboring sub-domains

(so-called ghost-cell data). Let $\bar{y}_m$ and $\bar{\dot{y}}_m$ denote y_m and $\dot{y}_m$ (respectively) augmented with those other components on which G_m depends. Then we have

$$G(t, y, \dot{y}) = [G_1(t, \bar{y}_1, \bar{\dot{y}}_1), G_2(t, \bar{y}_2, \bar{\dot{y}}_2), \ldots, G_M(t, \bar{y}_M, \bar{\dot{y}}_M)]^T , \qquad (4.1)$$

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

$$P = diag[P_1, P_2, \ldots, P_M] \qquad (4.2)$$

where

$$P_m \approx \partial G_m / \partial y_m + \alpha \partial G_m / \partial \dot{y}_m \qquad (4.3)$$

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

$$Px = b \qquad (4.4)$$

reduces to solving each of the equations

$$P_m x_m = b_m \qquad (4.5)$$

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 ex-
             ecution of the Gres function above, using the input vectors yy and yp.

Arguments    Nlocal      is the local vector length.

             tt          is the value of the independent variable.

             yy          is the dependent variable.

             yp          is the derivative of the dependent variable.

             user_data is a pointer to user data, the same as the user_data parameter passed to
                         IDASetUserData.

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

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

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

Besides the header files required for the integration of the DAE problem (see §4.3), to use the
IDABBDPRE module, the main program must include the header file idas_bbdpre.h which declares
the needed function prototypes.

The following is a summary of the usage of this module and describes the sequence of calls in
the user main program. Steps that are unchanged from the user main program presented in §4.4 are
grayed-out.

1. **Initialize MPI**

2. **Set problem dimensions etc.**

3. **Set vectors of initial values**

4. **Create** IDAS **object**

5. **Initialize** IDAS **solver**

6. **Specify integration tolerances**

7. **Create linear solver object**

   When creating the iterative linear solver object, specify the use of left preconditioning (PREC_LEFT)
   as IDAS only supports left preconditioning.

8. **Set linear solver optional inputs**

9. **Attach linear solver module**

10. Set optional inputs

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

11. **Initialize the** IDABBDPRE **preconditioner module**

    Specify the upper and lower bandwidths mudq, mldq and mukeep, mlkeep and call

    ```
    flag = IDABBDPrecInit(ida_mem, Nlocal, mudq, mldq,
                          mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);
    ```

    to allocate memory and initialize the internal preconditioner data. The last two arguments of IDABBDPrecInit are the two user-supplied functions described above.

12. Create nonlinear solver object

13. Attach nonlinear solver module

14. Set nonlinear solver optional inputs

15. Correct initial values

16. Specify rootfinding problem

17. Advance solution in time

18. **Get optional outputs**

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

19. Deallocate memory for solution vectors

20. Free solver memory

21. Free nonlinear solver memory

22. Free linear solver memory

23. Finalize MPI

The user-callable functions that initialize (step 11 above) or re-initialize the IDABBDPRE preconditioner module are described next.

IDABBDPrecInit

Call	`flag = IDABBDPrecInit(ida_mem, Nlocal, mudq, mldq,` `mukeep, mlkeep, dq_rel_yy, Gres, Gcomm);`
Description	The function IDABBDPrecInit initializes and allocates (internal) memory for the ID-ABBDPRE preconditioner.
Arguments	ida_mem (void *) pointer to the IDAS memory block.
	Nlocal (sunindextype) local vector dimension.
	mudq (sunindextype) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
	mldq (sunindextype) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
	mukeep (sunindextype) upper half-bandwidth of the retained banded approximate Jacobian block.

mlkeep	(`sunindextype`) lower half-bandwidth of the retained banded approximate Jacobian block.
dq_rel_yy	(`realtype`) the relative increment in components of y used in the difference quotient approximations. The default is `dq_rel_yy=` $\sqrt{\text{unit roundoff}}$, which can be specified by passing `dq_rel_yy=` 0.0.
Gres	(`IDABBDLocalFn`) the C function which computes the local residual approximation $G(t, y, \dot{y})$.
Gcomm	(`IDABBDCommFn`) the optional C function which performs all inter-process communication required for the computation of $G(t, y, \dot{y})$.

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

IDALS_SUCCESS	The call to `IDABBDPrecInit` was successful.
IDALS_MEM_NULL	The `ida_mem` pointer was NULL.
IDALS_MEM_FAIL	A memory allocation request has failed.
IDALS_LMEM_NULL	An IDALS linear solver memory was not attached.
IDALS_ILL_INPUT	The supplied vector implementation was not compatible with the block band preconditioner.

Notes If one of the half-bandwidths `mudq` or `mldq` to be used in the difference-quotient calculation of the approximate Jacobian is negative or exceeds the value `Nlocal`−1, it is replaced by 0 or `Nlocal`−1 accordingly.

The half-bandwidths `mudq` and `mldq` need not be the true half-bandwidths of the Jacobian of the local block of G, when smaller values may provide a greater efficiency.

Also, the half-bandwidths `mukeep` and `mlkeep` of the retained banded approximate Jacobian block may be even smaller, to reduce storage and computation costs further.

For all four half-bandwidths, the values need not be the same on every processor.

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 IDAS for a subsequent problem, a call to `IDABBDPrecReInit` can be made to change any of the following: the half-bandwidths `mudq` and `mldq` used in the difference-quotient Jacobian approximations, the relative increment `dq_rel_yy`, or one of the user-supplied functions `Gres` and `Gcomm`. If there is a change in any of the linear solver inputs, an additional call to the "Set" routines provided by the SUNLINSOL module, and/or one or more of the corresponding `IDASet***` functions, must also be made (in the proper order).

┌─────────────────┐
│ `IDABBDPrecReInit` │
└─────────────────┘

Call `flag = IDABBDPrecReInit(ida_mem, mudq, mldq, dq_rel_yy);`

Description The function `IDABBDPrecReInit` reinitializes the IDABBDPRE preconditioner.

Arguments

ida_mem	(`void *`) pointer to the IDAS memory block.
mudq	(`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.
mldq	(`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.
dq_rel_yy	(`realtype`) the relative increment in components of y used in the difference quotient approximations. The default is `dq_rel_yy =` $\sqrt{\text{unit roundoff}}$, which can be specified by passing `dq_rel_yy =` 0.0.

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

IDALS_SUCCESS	The call to `IDABBDPrecReInit` was successful.

	IDALS_MEM_NULL	The ida_mem pointer was NULL.
	IDALS_LMEM_NULL	An IDALS linear solver memory was not attached.
	IDALS_PMEM_NULL	The function IDABBDPrecInit was not previously called.

Notes   If one of the half-bandwidths mudq or mldq is negative or exceeds the value Nlocal−1, it is replaced by 0 or Nlocal−1, accordingly.

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 IDAS memory block.

             lenrwBBDP (long int) local number of real values in the IDABBDPRE workspace.

             leniwBBDP (long int) local number of integer values in the IDABBDPRE workspace.

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

             IDALS_SUCCESS   The optional output value has been successfully set.

             IDALS_MEM_NULL   The ida_mem pointer was NULL.

             IDALS_PMEM_NULL The IDABBDPRE preconditioner has not been initialized.

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

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

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 IDAS memory block.

             ngevalsBBDP (long int) the cumulative number of calls to the user Gres function.

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

             IDALS_SUCCESS   The optional output value has been successfully set.

             IDALS_MEM_NULL   The ida_mem pointer was NULL.

             IDALS_PMEM_NULL The IDABBDPRE preconditioner has not been initialized.

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

Chapter 5

Using IDAS for Forward Sensitivity Analysis

This chapter describes the use of IDAS to compute solution sensitivities using forward sensitivity analysis. One of our main guiding principles was to design the IDAS user interface for forward sensitivity analysis as an extension of that for IVP integration. Assuming a user main program and user-defined support routines for IVP integration have already been defined, in order to perform forward sensitivity analysis the user only has to insert a few more calls into the main program and (optionally) define an additional routine which computes the residuals for sensitivity systems (2.12). The only departure from this philosophy is due to the `IDAResFn` type definition (§4.6.1). Without changing the definition of this type, the only way to pass values of the problem parameters to the DAE residual function is to require the user data structure `user_data` to contain a pointer to the array of real parameters p.

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

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable routines and of the user-supplied routines that were not already described in Chapter 4.

5.1   A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) as an application of IDAS. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapter 9, 10, 11, and 12 for the specific name of the function to be called or macro to be referenced.

Differences between the user main program in §4.4 and the one below start only at step (16). Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

First, note that no additional header files need be included for forward sensitivity analysis beyond those for IVP solution (§4.4).

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

2. Set problem dimensions etc.

3. Set vectors of initial values

4. Create IDAS object

5. Initialize IDAS solver

6. Specify integration tolerances

7. Create matrix object

8. Create linear solver object

9. Set linear solver optional inputs

10. Attach linear solver module

11. Set optional inputs

12. Create nonlinear solver object

13. Attach nonlinear solver module

14. Set nonlinear solver optional inputs

15. Initialize quadrature problem, if not sensitivity-dependent

16. **Define the sensitivity problem**

 - Number of sensitivities (required)

   Set `Ns` = N_s, the number of parameters with respect to which sensitivities are to be computed.

 - Problem parameters (optional)

   If IDAS is to evaluate the residuals of the sensitivity systems, set `p`, an array of `Np` real parameters upon which the IVP depends. Only parameters with respect to which sensitivities are (potentially) desired need to be included. Attach `p` to the user data structure `user_data`. For example, `user_data->p = p;`

   If the user provides a function to evaluate the sensitivity residuals, `p` need not be specified.

 - Parameter list (optional)

   If IDAS is to evaluate the sensitivity residuals, set `plist`, an array of `Ns` integers to specify the parameters `p` with respect to which solution sensitivities are to be computed. If sensitivities with respect to the j-th parameter `p[j]` ($0 \leq$ `j` $<$ `Np`) are desired, set $\text{plist}_i = j$, for some $i = 0, \ldots, N_s - 1$.

   If `plist` is not specified, IDAS will compute sensitivities with respect to the first `Ns` parameters; i.e., $\text{plist}_i = i$ ($i = 0, \ldots, N_s - 1$).

   If the user provides a function to evaluate the sensitivity residuals, `plist` need not be specified.

 - Parameter scaling factors (optional)

   If IDAS is to estimate tolerances for the sensitivity solution vectors (based on tolerances for the state solution vector) or if IDAS is to evaluate the residuals of the sensitivity systems using the internal difference-quotient function, the results will be more accurate if order of magnitude information is provided.

   Set `pbar`, an array of `Ns` positive scaling factors. Typically, if $p_i \neq 0$, the value $\bar{p}_i = |p_{\text{plist}_i}|$ can be used.

   If `pbar` is not specified, IDAS will use $\bar{p}_i = 1.0$.

   If the user provides a function to evaluate the sensitivity residual and specifies tolerances for the sensitivity variables, `pbar` need not be specified.

   Note that the names for `p`, `pbar`, `plist`, as well as the field p of `user_data` are arbitrary, but they must agree with the arguments passed to `IDASetSensParams` below.

17. **Set sensitivity initial conditions**

    Set the Ns vectors yS0[i] and ypS0[i] of initial values for sensitivities (for $i = 0, \ldots,$ Ns -1), using the appropriate functions defined by the particular NVECTOR implementation chosen.

    First, create an array of Ns vectors by making the appropriate call

    yS0 = N_VCloneVectorArray_***(Ns, y0);

    or

    yS0 = N_VCloneVectorArrayEmpty_***(Ns, y0);

    Here the argument y0 serves only to provide the N_Vector type for cloning.

    Then, for each $i = 0, \ldots,$ Ns -1, load initial values for the i-th sensitivity vector yS0[i].

    Set the initial conditions for the Ns sensitivity derivative vectors ypS0 of $\dot{y}$ similarly.

18. **Activate sensitivity calculations**

    Call flag = IDASensInit(...); to activate forward sensitivity computations and allocate internal memory for IDAS related to sensitivity calculations (see §5.2.1).

19. **Set sensitivity tolerances**

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

20. **Set sensitivity analysis optional inputs**

    Call IDASetSens* routines to change from their default values any optional inputs that control the behavior of IDAS in computing forward sensitivities. See §5.2.7.

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

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

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

    where *** is the name of the nonlinear solver and ... are constructor specific arguments (see Chapter 12 for details).

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

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

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

    when using the IDA_SIMULTANEOUS corrector method or

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

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

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

    Call the appropriate set functions for the selected nonlinear solver module to change optional inputs specific to that nonlinear solver. These *must* be called after IDASensInit if using the default nonlinear solver or after attaching a new nonlinear solver to IDAS, otherwise the optional inputs will be overridden by IDAS defaults. See Chapter 12 for more information on optional inputs.

24. Correct initial values

25. Specify rootfinding problem

26. Advance solution in time

27. **Extract sensitivity solution**

    After each successful return from `IDASolve`, the solution of the original IVP is available in the `y` argument of `IDASolve`, while the sensitivity solution can be extracted into `yS` and `ypS` (which can be the same as `yS0` and `ypS0`, respectively) by calling one of the following routines: `IDAGetSens`, `IDAGetSens1`, `IDAGetSensDky` or `IDAGetSensDky1` (see §5.2.6).

28. Get optional outputs

29. Deallocate memory for solution vector

30. **Deallocate memory for sensitivity vectors**

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

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

    If `yS` was created from `realtype` arrays `yS_i`, it is the user's responsibility to also free the space for the arrays `yS_i`, and likewise for `ypS`.

31. **Free user data structure**

32. Free solver memory

33. Free nonlinear solver memory

34. Free vector specification memory

35. Free linear solver and matrix memory

36. Finalize MPI, if used

5.2   User-callable routines for forward sensitivity analysis

This section describes the IDAS functions, in addition to those presented in §4.5, that are called by the user to set up and solve a forward sensitivity problem.

5.2.1   Forward sensitivity initialization and deallocation functions

Activation of forward sensitivity computation is done by calling `IDASensInit`. The form of the call to this routine is as follows:

`IDASensInit`

Call	`flag = IDASensInit(ida_mem, Ns, ism, resS, yS0, ypS0);`
Description	The routine `IDASensInit` activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`Ns` (`int`) the number of sensitivities to be computed.
	`ism` (`int`) a flag used to select the sensitivity solution method. Its value can be either `IDA_SIMULTANEOUS` or `IDA_STAGGERED`:

- In the `IDA_SIMULTANEOUS` approach, the state and sensitivity variables are corrected at the same time. If the default Newton nonlinear solver is used, this amounts to performing a modified Newton iteration on the combined nonlinear system;

- In the `IDA_STAGGERED` approach, the correction step for the sensitivity variables takes place at the same time for all sensitivity equations, but only after the correction of the state variables has converged and the state variables have passed the local error test;

`resS`	(`IDASensResFn`) is the C function which computes the residual of the sensitivity DAE. For full details see §5.3.
`yS0`	(`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities of y.
`ypS0`	(`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities of $\dot{y}$.

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

`IDA_SUCCESS`	The call to `IDASensInit` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_MEM_FAIL`	A memory allocation request has failed.
`IDA_ILL_INPUT`	An input argument to `IDASensInit` has an illegal value.

Notes Passing `resS=NULL` indicates using the default internal difference quotient sensitivity residual routine.

If an error occurred, `IDASensInit` also prints an error message to the file specified by the optional input `errfp`.

F2003 Name `FIDASensInit`

In terms of the problem size N, number of sensitivity vectors N_s, and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value: `lenrw = lenrw` + (`maxord+5`)$N_s N$

- With `IDASensSVtolerances`: `lenrw = lenrw` $+ N_s N$

the size of the integer workspace is increased as follows:

- Base value: `leniw = leniw` + (`maxord+5`)$N_s N_i$

- With `IDASensSVtolerances`: `leniw = leniw` $+ N_s N_i$,

where N_i is the number of integer words in one `N_Vector`.

The routine `IDASensReInit`, useful during the solution of a sequence of problems of same size, reinitializes the sensitivity-related internal memory and must follow a call to `IDASensInit` (and maybe a call to `IDAReInit`). The number `Ns` of sensitivities is assumed to be unchanged since the call to `IDASensInit`. The call to the `IDASensReInit` function has the form:

`IDASensReInit`

Call	`flag = IDASensReInit(ida_mem, ism, yS0, ypS0);`
Description	The routine `IDASensReInit` reinitializes forward sensitivity computations.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`ism` (`int`) a flag used to select the sensitivity solution method. Its value can be either `IDA_SIMULTANEOUS` or `IDA_STAGGERED`.
	`yS0` (`N_Vector *`) a pointer to an array of `Ns` variables of type `N_Vector` containing the initial values of the sensitivities of y.

ypS0   (N_Vector *) a pointer to an array of Ns variables of type N_Vector containing
          the initial values of the sensitivities of $\dot{y}$.

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

IDA_SUCCESS   The call to IDAReInit was successful.

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

IDA_NO_SENS   Memory space for sensitivity integration was not allocated through a
               previous call to IDASensInit.

IDA_ILL_INPUT An input argument to IDASensReInit has an illegal value.

IDA_MEM_FAIL   A memory allocation request has failed.

Notes   All arguments of IDASensReInit are the same as those of IDASensInit.

              If an error occurred, IDASensReInit also prints an error message to the file specified
              by the optional input errfp.

F2003 Name FIDASensReInit

To deallocate all forward sensitivity-related memory (allocated in a prior call to IDASensInit), the
user must call

| IDASensFree |

Call   IDASensFree(ida_mem);

Description   The function IDASensFree frees the memory allocated for forward sensitivity compu-
              tations by a previous call to IDASensInit.

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

Return value The function IDASensFree has no return value.

Notes   In general, IDASensFree need not be called by the user as it is invoked automatically
              by IDAFree.

              After a call to IDASensFree, forward sensitivity computations can be reactivated only
              by calling IDASensInit again.

F2003 Name FIDASensFree

To activate and deactivate forward sensitivity calculations for successive IDAS runs, without having
to allocate and deallocate memory, the following function is provided:

| IDASensToggleOff |

Call   IDASensToggleOff(ida_mem);

Description   The function IDASensToggleOff deactivates forward sensitivity calculations. It does
              not deallocate sensitivity-related memory.

Arguments   ida_mem (void *) pointer to the memory previously allocated by IDAInit.

Return value The return value flag of IDASensToggle is one of:

IDA_SUCCESS   IDASensToggleOff was successful.

IDA_MEM_NULL ida_mem was NULL.

Notes   Since sensitivity-related memory is not deallocated, sensitivities can be reactivated at
              a later time (using IDASensReInit).

F2003 Name FIDASensToggleOff

5.2.2 Forward sensitivity tolerance specification functions

One of the following three functions must be called to specify the integration tolerances for sensitivities.
Note that this call must be made after the call to IDASensInit.

$\boxed{\texttt{IDASensSStolerances}}$

Call	`flag = IDASensSStolerances(ida_mem, reltolS, abstolS);`
Description	The function `IDASensSStolerances` specifies scalar relative and absolute tolerances.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`reltolS` (`realtype`) is the scalar relative error tolerance.
	`abstolS` (`realtype*`) is a pointer to an array of length `Ns` containing the scalar absolute error tolerances.
Return value	The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASStolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_SENS`	The sensitivity allocation function `IDASensInit` has not been called.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name	`FIDASensSStolerances`

$\boxed{\texttt{IDASensSVtolerances}}$

Call	`flag = IDASensSVtolerances(ida_mem, reltolS, abstolS);`
Description	The function `IDASensSVtolerances` specifies scalar relative tolerance and vector absolute tolerances.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`reltolS` (`realtype`) is the scalar relative error tolerance.
	`abstolS` (`N_Vector*`) is an array of `Ns` variables of type `N_Vector`. The `N_Vector` from `abstolS[is]` specifies the vector tolerances for `is`-th sensitivity.
Return value	The return flag `flag` (of type `int`) will be one of the following:

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

Notes	This choice of tolerances is important when the absolute error tolerance needs to be different for each component of any vector `yS[i]`.
F2003 Name	`FIDASensSVtolerances`

$\boxed{\texttt{IDASensEEtolerances}}$

Call	`flag = IDASensEEtolerances(ida_mem);`
Description	When `IDASensEEtolerances` is called, IDAS will estimate tolerances for sensitivity variables based on the tolerances supplied for states variables and the scaling factors $\bar{p}$.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
Return value	The return flag `flag` (of type `int`) will be one of the following:

`IDA_SUCCESS`	The call to `IDASensEEtolerances` was successful.
`IDA_MEM_NULL`	The IDAS memory block was not initialized through a previous call to `IDACreate`.
`IDA_NO_SENS`	The sensitivity allocation function `IDASensInit` has not been called.

F2003 Name	`FIDASensEEtolerances`

5.2.3 Forward sensitivity nonlinear solver interface functions

As in the pure DAE case, when computing solution sensitivities using forward sensitivitiy analysis IDAS uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §12.3) by default. To specify a different nonlinear solver in IDAS, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to IDAS by calling either IDASetNonlinearSolverSensSim when using the IDA_SIMULTANEOUS corrector option, or IDASetNonlinearSolver (see §4.5.4) and IDASetNonlinearSolverSensStg when using the IDA_STAGGERED corrector option, as documented below.

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

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

IDASetNonlinearSolverSensSim

Call   flag = IDASetNonlinearSolverSensSim(ida_mem, NLS);

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

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

                NLS   (SUNNonlinearSolver) SUNNONLINSOL object to use for solving nonlinear systems.

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

                IDA_SUCCESS   The nonlinear solver was successfully attached.

                IDA_MEM_NULL   The ida_mem pointer is NULL.

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

F2003 Name   FIDASetNonlinearSolverSensSim

IDASetNonlinearSolverSensStg

Call   flag = IDASetNonlinearSolverSensStg(ida_mem, NLS);

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

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

                NLS   (SUNNonlinearSolver) SUNNONLINSOL object to use for solving nonlinear systems.

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

                IDA_SUCCESS   The nonlinear solver was successfully attached.

                IDA_MEM_NULL   The ida_mem pointer is NULL.

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

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

F2003 Name   FIDASetNonlinearSolverSensStg

5.2.4   Forward sensitivity initial condition calculation function

IDACalcIC also calculates corrected initial conditions for sensitivity variables of a DAE system. When used for initial conditions calculation of the forward sensitivities, IDACalcIC must be preceded by successful calls to IDASensInit (or IDASensReInit) and should precede the call(s) to IDASolve. For restrictions that apply for initial conditions calculation of the state variables, see §4.5.5.

Calling IDACalcIC is optional. It is only necessary when the initial conditions do not satisfy the sensitivity systems. Even if forward sensitivity analysis was enabled, the call to the initial conditions calculation function IDACalcIC is exactly the same as for state variables.

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

See §4.5.5 for a list of possible return values.

5.2.5   IDAS solver function

Even if forward sensitivity analysis was enabled, the call to the main solver function IDASolve is exactly the same as in §4.5.7. However, in this case the return value flag can also be one of the following:

IDA_SRES_FAIL   The sensitivity residual function failed in an unrecoverable manner.

IDA_REP_SRES_ERR The user's residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.

5.2.6   Forward sensitivity extraction functions

If forward sensitivity computations have been initialized by a call to IDASensInit, or reinitialized by a call to IDASensReInit, then IDAS computes both a solution and sensitivities at time t. However, IDASolve will still return only the solutions y and $\dot{y}$ in yret and ypret, respectively. Solution sensitivities can be obtained through one of the following functions:

IDAGetSens

Call   flag = IDAGetSens(ida_mem, &tret, yS);

Description   The function IDAGetSens returns the sensitivity solution vectors after a successful return from IDASolve.

Arguments   ida_mem (void *) pointer to the memory previously allocated by IDAInit.

              tret   (realtype) the time reached by the solver (output).

              yS   (N_Vector *) the array of Ns computed forward sensitivity vectors.

Return value The return value flag of IDAGetSens is one of:

           IDA_SUCCESS   IDAGetSens was successful.

           IDA_MEM_NULL ida_mem was NULL.

           IDA_NO_SENS   Forward sensitivity analysis was not initialized.

           IDA_BAD_DKY   yS is NULL.

Notes   Note that the argument `tret` is an output for this function. Its value will be the same
               as that returned at the last `IDASolve` call.

F2003 Name   `FIDAGetSens`

The function `IDAGetSensDky` computes the `k`-th derivatives of the interpolating polynomials for the
sensitivity variables at time `t`. This function is called by `IDAGetSens` with `k = 0`, but may also be
called directly by the user.

| `IDAGetSensDky` |

Call   `flag = IDAGetSensDky(ida_mem, t, k, dkyS);`

Description   The function `IDAGetSensDky` returns derivatives of the sensitivity solution vectors after
               a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

               `t`   (`realtype`) specifies the time at which sensitivity information is requested.
                          The time `t` must fall within the interval defined by the last successful step
                          taken by IDAS.

               `k`   (`int`) order of derivatives. `k` must be in the range $0, 1, ..., klast$ where $klast$ is
                          the method order of the last successful step.

               `dkyS`   (`N_Vector *`) array of `Ns` vectors containing the derivatives on output. The
                          space for `dkyS` must be allocated by the user.

Return value   The return value `flag` of `IDAGetSensDky` is one of:

               `IDA_SUCCESS`   `IDAGetSensDky` succeeded.

               `IDA_MEM_NULL` `ida_mem` was NULL.

               `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

               `IDA_BAD_DKY`   `dkyS` or one of the vectors `dkyS[i]` is NULL.

               `IDA_BAD_K`   `k` is not in the range $0, 1, ..., klast$.

               `IDA_BAD_T`   The time `t` is not in the allowed range.

F2003 Name   `FIDAGetSensDky`

Forward sensitivity solution vectors can also be extracted separately for each parameter in turn
through the functions `IDAGetSens1` and `IDAGetSensDky1`, defined as follows:

| `IDAGetSens1` |

Call   `flag = IDAGetSens1(ida_mem, &tret, is, yS);`

Description   The function `IDAGetSens1` returns the `is`-th sensitivity solution vector after a successful
               return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

               `tret`   (`realtype *`) the time reached by the solver (output).

               `is`   (`int`) specifies which sensitivity vector is to be returned ($0 \leq$ `is` $< N_s$).

               `yS`   (`N_Vector`) the computed forward sensitivity vector.

Return value   The return value `flag` of `IDAGetSens1` is one of:

               `IDA_SUCCESS`   `IDAGetSens1` was successful.

               `IDA_MEM_NULL` `ida_mem` was NULL.

               `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

               `IDA_BAD_IS`   The index `is` is not in the allowed range.

               `IDA_BAD_DKY`   `yS` is NULL.

               `IDA_BAD_T`   The time `t` is not in the allowed range.

Notes   Note that the argument `tret` is an output for this function. Its value will be the same
               as that returned at the last `IDASolve` call.

F2003 Name   `FIDAGetSens1`

| IDAGetSensDky1 |

Call	`flag = IDAGetSensDky1(ida_mem, t, k, is, dkyS);`
Description	The function `IDAGetSensDky1` returns the `k`-th derivative of the `is`-th sensitivity solution vector after a successful return from `IDASolve`.
Arguments	`ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

      `t`   (`realtype`) specifies the time at which sensitivity information is requested. The time `t` must fall within the interval defined by the last successful step taken by IDAS.

      `k`   (`int`) order of derivative. `k` must be in the range $0, 1, ..., klast$ where $klast$ is the method order of the last successful step.

      `is`   (`int`) specifies the sensitivity derivative vector to be returned ($0 \leq$ `is` $< N_s$).

      `dkyS` (`N_Vector`) the vector containing the derivative on output. The space for `dkyS` must be allocated by the user.

Return value	The return value `flag` of `IDAGetSensDky1` is one of:

      `IDA_SUCCESS`   `IDAGetQuadDky1` succeeded.

      `IDA_MEM_NULL` `ida_mem` was NULL.

      `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

      `IDA_BAD_DKY`   `dkyS` is NULL.

      `IDA_BAD_IS`   The index `is` is not in the allowed range.

      `IDA_BAD_K`   `k` is not in the range $0, 1, ..., klast$.

      `IDA_BAD_T`   The time `t` is not in the allowed range.

F2003 Name	`FIDAGetSensDky1`

5.2.7 Optional inputs for forward sensitivity analysis

Optional input variables that control the computation of sensitivities can be changed from their default values through calls to `IDASetSens*` functions. Table 5.1 lists all forward sensitivity optional input functions in IDAS which are described in detail in the remainder of this section.

    We note that, on an error return, all of the optional input functions 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 `IDASetSens***` function can be made from the user's calling program at any time and, if successful, takes effect immediately.

| IDASetSensParams |

Call	`flag = IDASetSensParams(ida_mem, p, pbar, plist);`
Description	The function `IDASetSensParams` specifies problem parameter information for sensitivity calculations.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.

      `p`   (`realtype *`) a pointer to the array of real problem parameters used to evaluate $F(t, y, \dot{y}, p)$. If non-NULL, `p` must point to a field in the user's data structure `user_data` passed to the user's residual function. (See §5.1).

Table 5.1: Forward sensitivity optional inputs

Optional input	Routine name	Default
Sensitivity scaling factors	`IDASetSensParams`	NULL
DQ approximation method	`IDASetSensDQMethod`	centered,0.0
Error control strategy	`IDASetSensErrCon`	SUNFALSE
Maximum no. of nonlinear iterations	`IDASetSensMaxNonlinIters`	4

pbar   (`realtype *`) an array of `Ns` positive scaling factors. If non-NULL, `pbar` must have all its components > 0.0. (See §5.1).

plist   (`int *`) an array of `Ns` non-negative indices to specify which components of `p` to use in estimating the sensitivity equations. If non-NULL, `plist` must have all components ≥ 0. (See §5.1).

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

      IDA_SUCCESS   The optional value has been successfully set.

      IDA_MEM_NULL   The `ida_mem` pointer is NULL.

      IDA_NO_SENS   Forward sensitivity analysis was not initialized.

      IDA_ILL_INPUT   An argument has an illegal value.

Notes   This function must be preceded by a call to `IDASensInit`.

F2003 Name   `FIDASetSensParams`

IDASetSensDQMethod

Call   `flag = IDASetSensDQMethod(ida_mem, DQtype, DQrhomax);`

Description   The function `IDASetSensDQMethod` specifies the difference quotient strategy in the case in which the residual of the sensitivity equations are to be computed by IDAS.

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

      `DQtype` (`int`) specifies the difference quotient type and can be either `IDA_CENTERED` or `IDA_FORWARD`.

      `DQrhomax` (`realtype`) positive value of the selection parameter used in deciding switching between a simultaneous or separate approximation of the two terms in the sensitivity residual.

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

      IDA_SUCCESS   The optional value has been successfully set.

      IDA_MEM_NULL   The `ida_mem` pointer is NULL.

      IDA_ILL_INPUT   An argument has an illegal value.

Notes   If `DQrhomax` $= 0.0$, then no switching is performed. The approximation is done simultaneously using either centered or forward finite differences, depending on the value of `DQtype`. For values of `DQrhomax` ≥ 1.0, the simultaneous approximation is used whenever the estimated finite difference perturbations for states and parameters are within a factor of `DQrhomax`, and the separate approximation is used otherwise. Note that a value `DQrhomax` < 1.0 will effectively disable switching. See §2.5 for more details.

      The default value are `DQtype`=`IDA_CENTERED` and `DQrhomax`$= 0.0$.

F2003 Name   `FIDASetSensDQMethod`

IDASetSensErrCon

Call   `flag = IDASetSensErrCon(ida_mem, errconS);`

Description   The function `IDASetSensErrCon` specifies the error control strategy for sensitivity variables.

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

      `errconS` (`booleantype`) specifies whether sensitivity variables are included (`SUNTRUE`) or not (`SUNFALSE`) in the error control mechanism.

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

      IDA_SUCCESS   The optional value has been successfully set.

      IDA_MEM_NULL   The `ida_mem` pointer is NULL.

Notes   By default, `errconS` is set to `SUNFALSE`. If `errconS=SUNTRUE` then both state variables
             and sensitivity variables are included in the error tests. If `errconS=SUNFALSE` then
             the sensitivity variables are excluded from the error tests. Note that, in any event, all
             variables are considered in the convergence tests.

F2003 Name `FIDASetSensErrCon`

| `IDASetSensMaxNonlinIters` |

Call   `flag = IDASetSensMaxNonlinIters(ida_mem, maxcorS);`

Description The function `IDASetSensMaxNonlinIters` specifies the maximum number of nonlinear
             solver iterations for sensitivity variables per step.

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

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

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

Notes   The default value is 4.

F2003 Name `FIDASetSensMaxNonlinIters`

5.2.8   Optional outputs for forward sensitivity analysis

5.2.8.1   Main solver optional output functions

Optional output functions that return statistics and solver performance information related to forward
sensitivity computations are listed in Table 5.2 and described in detail in the remainder of this section.

| `IDAGetSensNumResEvals` |

Call   `flag = IDAGetSensNumResEvals(ida_mem, &nfSevals);`

Description The function `IDAGetSensNumResEvals` returns the number of calls to the sensitivity
             residual function.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block.
             `nfSevals` (`long int`) number of calls to the sensitivity residual function.

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

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

Table 5.2: Forward sensitivity optional outputs

Optional output	Routine name
No. of calls to sensitivity residual function	`IDAGetSensNumResEvals`
No. of calls to residual function for sensitivity	`IDAGetNumResEvalsSens`
No. of sensitivity local error test failures	`IDAGetSensNumErrTestFails`
No. of calls to lin. solv. setup routine for sens.	`IDAGetSensNumLinSolvSetups`
Sensitivity-related statistics as a group	`IDAGetSensStats`
Error weight vector for sensitivity variables	`IDAGetSensErrWeights`
No. of sens. nonlinear solver iterations	`IDAGetSensNumNonlinSolvIters`
No. of sens. convergence failures	`IDAGetSensNumNonlinSolvConvFails`
Sens. nonlinear solver statistics as a group	`IDAGetSensNonlinSolvStats`

IDA_MEM_NULL The ida_mem pointer is NULL.

IDA_NO_SENS   Forward sensitivity analysis was not initialized.

F2003 Name   FIDAGetSensNumResEvals

| IDAGetNumResEvalsSens |

Call   flag = IDAGetNumResEvalsSens(ida_mem, &nfevalsS);

Description   The function IDAGetNumResEvalsSEns returns the number of calls to the user's residual
              function due to the internal finite difference approximation of the sensitivity residuals.

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

              nfevalsS (long int) number of calls to the user residual function for sensitivity resid-
                       uals.

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

              IDA_SUCCESS   The optional output value has been successfully set.

              IDA_MEM_NULL The ida_mem pointer is NULL.

              IDA_NO_SENS   Forward sensitivity analysis was not initialized.

Notes   This counter is incremented only if the internal finite difference approximation routines
              are used for the evaluation of the sensitivity residuals.

F2003 Name   FIDAGetNumResEvalsSens

| IDAGetSensNumErrTestFails |

Call   flag = IDAGetSensNumErrTestFails(ida_mem, &nSetfails);

Description   The function IDAGetSensNumErrTestFails returns the number of local error test fail-
              ures for the sensitivity variables that have occurred.

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

              nSetfails (long int) number of error test failures.

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

              IDA_SUCCESS   The optional output value has been successfully set.

              IDA_MEM_NULL The ida_mem pointer is NULL.

              IDA_NO_SENS   Forward sensitivity analysis was not initialized.

Notes   This counter is incremented only if the sensitivity variables have been included in the
              error test (see IDASetSensErrCon in §5.2.7). Even in that case, this counter is not
              incremented if the ism=IDA_SIMULTANEOUS sensitivity solution method has been used.

F2003 Name   FIDAGetSensNumErrTestFails

| IDAGetSensNumLinSolvSetups |

Call   flag = IDAGetSensNumLinSolvSetups(ida_mem, &nlinsetupsS);

Description   The function IDAGetSensNumLinSolvSetups returns the number of calls to the linear
              solver setup function due to forward sensitivity calculations.

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

              nlinsetupsS (long int) number of calls to the linear solver setup function.

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

              IDA_SUCCESS   The optional output value has been successfully set.

              IDA_MEM_NULL The ida_mem pointer is NULL.

              IDA_NO_SENS   Forward sensitivity analysis was not initialized.

Notes   This counter is incremented only if a nonlinear solver requiring linear solves has been used and staggered sensitivity solution method (`ism=IDA_STAGGERED`) was specified in the call to `IDASensInit` (see §5.2.1).

F2003 Name   `FIDAGetSensNumLinSolvSetups`

`IDAGetSensStats`

Call   `flag = IDAGetSensStats(ida_mem, &nfSevals, &nfevalsS, &nSetfails,`
                         `&nlinsetupsS);`

Description   The function `IDAGetSensStats` returns all of the above sensitivity-related solver statistics as a group.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block.
             `nfSevals` (`long int`) number of calls to the sensitivity residual function.
             `nfevalsS` (`long int`) number of calls to the user-supplied residual function.
             `nSetfails` (`long int`) number of error test failures.
             `nlinsetupsS` (`long int`) number of calls to the linear solver setup function.

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

         `IDA_SUCCESS`   The optional output values have been successfully set.
         `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
         `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

F2003 Name   `FIDAGetSensStats`

`IDAGetSensErrWeights`

Call   `flag = IDAGetSensErrWeights(ida_mem, eSweight);`

Description   The function `IDAGetSensErrWeights` returns the sensitivity error weight vectors at the current time. These are the reciprocals of the W_i of (2.7) for the sensitivity variables.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block.
             `eSweight` (`N_Vector_S`) pointer to the array of error weight vectors.

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

         `IDA_SUCCESS`   The optional output value has been successfully set.
         `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
         `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

Notes   The user must allocate memory for `eweightS`.

F2003 Name   `FIDAGetSensErrWeights`

`IDAGetSensNumNonlinSolvIters`

Call   `flag = IDAGetSensNumNonlinSolvIters(ida_mem, &nSniters);`

Description   The function `IDAGetSensNumNonlinSolvIters` returns the number of nonlinear iterations performed for sensitivity calculations.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block.
             `nSniters` (`long int`) number of nonlinear iterations performed.

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

         `IDA_SUCCESS`   The optional output value has been successfully set.
         `IDA_MEM_NULL` The `ida_mem` pointer is `NULL`.
         `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

                IDA_MEM_FAIL The SUNNONLINSOL module is NULL.

Notes   This counter is incremented only if `ism` was IDA_STAGGERED in the call to `IDASensInit` (see §5.2.1).

F2003 Name   `FIDAGetSensNumNonlinSolvIters`

`IDAGetSensNumNonlinSolvConvFails`

Call   `flag = IDAGetSensNumNonlinSolvConvFails(ida_mem, &nSncfails);`

Description The function `IDAGetSensNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred for sensitivity calculations.

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

              `nSncfails` (`long int`) number of nonlinear convergence failures.

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

              IDA_SUCCESS   The optional output value has been successfully set.

              IDA_MEM_NULL The `ida_mem` pointer is NULL.

              IDA_NO_SENS   Forward sensitivity analysis was not initialized.

Notes   This counter is incremented only if `ism` was IDA_STAGGERED in the call to `IDASensInit` (see §5.2.1).

F2003 Name   `FIDAGetSensNumNonlinSolvConvFails`

`IDAGetSensNonlinSolvStats`

Call   `flag = IDAGetSensNonlinSolvStats(ida_mem, &nSniters, &nSncfails);`

Description The function `IDAGetSensNonlinSolvStats` returns the sensitivity-related nonlinear solver statistics as a group.

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

              `nSniters` (`long int`) number of nonlinear iterations performed.

              `nSncfails` (`long int`) number of nonlinear convergence failures.

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

              IDA_SUCCESS   The optional output values have been successfully set.

              IDA_MEM_NULL The `ida_mem` pointer is NULL.

              IDA_NO_SENS   Forward sensitivity analysis was not initialized.

              IDA_MEM_FAIL The SUNNONLINSOL module is NULL.

F2003 Name   `FIDAGetSensNonlinSolvStats`

5.2.8.2   Initial condition calculation optional output functions

The sensitivity consistent initial conditions found by IDAS (after a successful call to `IDACalcIC`) can be obtained by calling the following function:

`IDAGetSensConsistentIC`

Call   `flag = IDAGetSensConsistentIC(ida_mem, yyS0_mod, ypS0_mod);`

Description The function `IDAGetSensConsistentIC` returns the corrected initial conditions calculated by `IDACalcIC` for sensitivities variables.

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

              `yyS0_mod` (`N_Vector *`) a pointer to an array of `Ns` vectors containing consistent sensitivity vectors.

ypS0_mod (N_Vector *) a pointer to an array of Ns vectors containing consistent sensitivity derivative vectors.

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

IDA_SUCCESS   IDAGetSensConsistentIC succeeded.

IDA_MEM_NULL   The ida_mem pointer is NULL.

IDA_NO_SENS   The function IDASensInit has not been previously called.

IDA_ILL_INPUT IDASolve has been already called.

Notes   If the consistent sensitivity vectors or consistent derivative vectors are not desired, pass NULL for the corresponding argument.

The user must allocate space for yyS0_mod and ypS0_mod (if not NULL).

F2003 Name FIDAGetSensConsistentIC

5.3 User-supplied routines for forward sensitivity analysis

In addition to the required and optional user-supplied routines described in §4.6, when using IDAS for forward sensitivity analysis, the user has the option of providing a routine that calculates the residual of the sensitivity equations (2.12).

By default, IDAS uses difference quotient approximation routines for the residual of the sensitivity equations. However, IDAS allows the option for user-defined sensitivity residual routines (which also provides a mechanism for interfacing IDAS to routines generated by automatic differentiation).

The user may provide the residuals of the sensitivity equations (2.12), for all sensitivity parameters at once, through a function of type IDASensResFn defined by:

IDASensResFn

Definition   typedef int (*IDASensResFn)(int Ns, realtype t,
                                          N_Vector yy, N_Vector yp, N_Vector resval,
                                          N_Vector *yS, N_Vector *ypS,
                                          N_Vector *resvalS, void *user_data,
                                          N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);

Purpose   This function computes the sensitivity residual for all sensitivity equations. It must compute the vectors $(\partial F/\partial y)s_i(t) + (\partial F/\partial \dot{y})\dot{s}_i(t) + (\partial F/\partial p_i)$ and store them in resvalS[i].

Arguments   Ns   is the number of sensitivities.

t   is the current value of the independent variable.

yy   is the current value of the state vector, $y(t)$.

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

resval   contains the current value F of the original DAE residual.

yS   contains the current values of the sensitivities s_i.

ypS   contains the current values of the sensitivity derivatives $\dot{s}_i$.

resvalS   contains the output sensitivity residual vectors. Memory allocation for resvalS is handled within IDAS.

user_data is a pointer to user data.

tmp1

tmp2

tmp3   are N_Vectors of length N which can be used as temporary storage.

Return value An IDASensResFn should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and IDA_SRES_FAIL is returned).

Notes   There is one situation in which recovery is not possible even if IDASensResFn function returns a recoverable error flag. That is when this occurs at the very first call to the IDASensResFn, in which case IDAS returns IDA_FIRST_RES_FAIL.

5.4   Integration of quadrature equations depending on forward sensitivities

IDAS provides support for integration of quadrature equations that depends not only on the state variables but also on forward sensitivities.

The following is an overview of the sequence of calls in a user's main program in this situation. Steps that are unchanged from the skeleton program presented in §5.1 are grayed out. See also §4.7.

1. Initialize parallel or multi-threaded environment

2. Set problem dimensions, etc.

3. Set vectors of initial values

4. Create IDAS object

5. Initialize IDAS solver

6. Specify integration tolerances

7. Create matrix object

8. Create linear solver object

9. Set linear solver optional inputs

10. Attach linear solver module

11. Set optional inputs

12. Create nonlinear solver object

13. Attach nonlinear solver module

14. Set nonlinear solver optional inputs

15. Initialize sensitivity-independent quadrature problem

16. Define the sensitivity problem

17. Set sensitivity initial conditions

18. Activate sensitivity calculations

19. Set sensitivity tolerances

20. Set sensitivity analysis optional inputs

21. Create sensitivity nonlinear solver object

22. Attach the sensitvity nonlinear solver module

23. Set sensitivity nonlinear solver optional inputs

24. **Set vector of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.

25. **Initialize sensitivity-dependent quadrature integration**

    Call `IDAQuadSensInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §5.4.1 for details.

26. **Set optional inputs for sensitivity-dependent quadrature integration**

   Call `IDASetQuadSensErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `IDAQuadSens*tolerances` functions must be called to specify the integration tolerances for quadrature variables. See §5.4.4 for details.

27. Advance solution in time

28. **Extract sensitivity-dependent quadrature variables**

   Call `IDAGetQuadSens`, `IDAGetQuadSens1`, `IDAGetQuadSensDky` or `IDAGetQuadSensDky1` to obtain the values of the quadrature variables or their derivatives at the current time. See §5.4.3 for details.

29. Get optional outputs

30. Extract sensitivity solution

31. **Get sensitivity-dependent quadrature optional outputs**

   Call `IDAGetQuadSens*` functions to obtain optional output related to the integration of sensitivity-dependent quadratures. See §5.4.5 for details.

32. Deallocate memory for solutions vector

33. Deallocate memory for sensitivity vectors

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

35. Free solver memory

36. Free nonlinear solver memory

37. Free vector specification memory

38. Free linear solver and matrix memory

39. Finalize MPI, if used

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

5.4.1   Sensitivity-dependent quadrature initialization and deallocation

The function `IDAQuadSensInit` activates integration of quadrature equations depending on sensitivities and allocates internal memory related to these calculations. If `rhsQS` is input as `NULL`, then IDAS uses an internal function that computes difference quotient approximations to the functions $\bar{q}_i = (\partial q/\partial y)s_i + (\partial q/\partial \dot{y})\dot{s}_i + \partial q/\partial p_i$, in the notation of (2.10). The form of the call to this function is as follows:

`IDAQuadSensInit`

Call	`flag = IDAQuadSensInit(ida_mem, rhsQS, yQS0);`
Description	The function `IDAQuadSensInit` provides required problem specifications, allocates internal memory, and initializes quadrature integration.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`rhsQS` (`IDAQuadSensRhsFn`) is the C function which computes f_{QS}, the right-hand side of the sensitivity-dependent quadrature equations (for full details see §5.4.6).
	`yQS0` (`N_Vector *`) contains the initial values of sensitivity-dependent quadratures.

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

IDA_SUCCESS	The call to `IDAQuadSensInit` was successful.
IDA_MEM_NULL	The IDAS memory was not initialized by a prior call to `IDACreate`.
IDA_MEM_FAIL	A memory allocation request failed.
IDA_NO_SENS	The sensitivities were not initialized by a prior call to `IDASensInit`.
IDA_ILL_INPUT	The parameter `yQS0` is NULL.

Notes   Before calling `IDAQuadSensInit`, the user must enable the sensitivites by calling `IDASensInit`.

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

F2003 Name `FIDAQuadSensInit`

In terms of the number of quadrature variables N_q and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value: $\texttt{lenrw} = \texttt{lenrw} + (\texttt{maxord+5})N_q$

- If `IDAQuadSensSVtolerances` is called: $\texttt{lenrw} = \texttt{lenrw} + N_q N_s$

and the size of the integer workspace is increased as follows:

- Base value: $\texttt{leniw} = \texttt{leniw} + (\texttt{maxord+5})N_q$

- If `IDAQuadSensSVtolerances` is called: $\texttt{leniw} = \texttt{leniw} + N_q N_s$

The function `IDAQuadSensReInit`, useful during the solution of a sequence of problems of same size, reinitializes the quadrature related internal memory and must follow a call to `IDAQuadSensInit`. The number `Nq` of quadratures as well as the number `Ns` of sensitivities are assumed to be unchanged from the prior call to `IDAQuadSensInit`. The call to the `IDAQuadSensReInit` function has the form:

IDAQuadSensReInit

Call   `flag = IDAQuadSensReInit(ida_mem, yQS0);`

Description The function `IDAQuadSensReInit` provides required problem specifications and reinitializes the sensitivity-dependent quadrature integration.

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

`yQS0`   (`N_Vector *`) contains the initial values of sensitivity-dependent quadratures.

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

IDA_SUCCESS	The call to `IDAQuadSensReInit` was successful.
IDA_MEM_NULL	The IDAS memory was not initialized by a prior call to `IDACreate`.
IDA_NO_SENS	Memory space for the sensitivity calculation was not allocated by a prior call to `IDASensInit`.
IDA_NO_QUADSENS	Memory space for the sensitivity quadratures integration was not allocated by a prior call to `IDAQuadSensInit`.
IDA_ILL_INPUT	The parameter `yQS0` is NULL.

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

F2003 Name `FIDAQuadSensReInit`

IDAQuadSensFree

Call   `IDAQuadSensFree(ida_mem);`

Description   The function `IDAQuadSensFree` frees the memory allocated for sensitivity quadrature integration.

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

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

Notes   In general, `IDAQuadSensFree` need not be called by the user as it is called automatically by `IDAFree`.

F2003 Name   `FIDAQuadSensFree`

5.4.2   IDAS solver function

Even if quadrature integration was enabled, the call to the main solver function `IDASolve` is exactly the same as in §4.5.7. However, in this case the return value `flag` can also be one of the following:

`IDA_QSRHS_FAIL`   The sensitivity quadrature right-hand side function failed in an unrecoverable manner.

`IDA_FIRST_QSRHS_ERR` The sensitivity quadrature right-hand side function failed at the first call.

`IDA_REP_QSRHS_ERR`   Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. The `IDA_REP_RES_ERR` will also be returned if the quadrature right-hand side function had repeated recoverable errors during the estimation of an initial step size (assuming the sensitivity quadrature variables are included in the error tests).

5.4.3   Sensitivity-dependent quadrature extraction functions

If sensitivity-dependent quadratures have been initialized by a call to `IDAQuadSensInit`, or reinitialized by a call to `IDAQuadSensReInit`, then IDAS computes a solution, sensitivities, and quadratures depending on sensitivities at time `t`. However, `IDASolve` will still return only the solutions y and $\dot{y}$. Sensitivity-dependent quadratures can be obtained using one of the following functions:

IDAGetQuadSens

Call   `flag = IDAGetQuadSens(ida_mem, &tret, yQS);`

Description   The function `IDAGetQuadSens` returns the quadrature sensitivity solution vectors after a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.
              `tret`   (`realtype`) the time reached by the solver (output).
              `yQS`   (`N_Vector *`) array of `Ns` computed sensitivity-dependent quadrature vectors. This array of vectors must be allocated by the user.

Return value The return value `flag` of `IDAGetQuadSens` is one of:

              `IDA_SUCCESS`   `IDAGetQuadSens` was successful.
              `IDA_MEM_NULL`   `ida_mem` was NULL.
              `IDA_NO_SENS`   Sensitivities were not activated.
              `IDA_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.
              `IDA_BAD_DKY`   `yQS` or one of the `yQS[i]` is NULL.

F2003 Name   `FIDAGetQuadSens`

The function `IDAGetQuadSensDky` computes the `k`-th derivatives of the interpolating polynomials for the sensitivity-dependent quadrature variables at time `t`. This function is called by `IDAGetQuadSens` with `k = 0`, but may also be called directly by the user.

IDAGetQuadSensDky

Call   `flag = IDAGetQuadSensDky(ida_mem, t, k, dkyQS);`

Description   The function `IDAGetQuadSensDky` returns derivatives of the quadrature sensitivities solution vectors after a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

          `t`   (`realtype`) the time at which information is requested. The time `t` must fall within the interval defined by the last successful step taken by IDAS.

          `k`   (`int`) order of the requested derivative. `k` must be in the range $0, 1, ..., klast$ where $klast$ is the method order of the last successful step.

          `dkyQS`   (`N_Vector *`) array of `Ns` vectors containing the derivatives. This vector array must be allocated by the user.

Return value The return value `flag` of `IDAGetQuadSensDky` is one of:

          `IDA_SUCCESS`   `IDAGetQuadSensDky` succeeded.

          `IDA_MEM_NULL`   `ida_mem` was NULL.

          `IDA_NO_SENS`   Sensitivities were not activated.

          `IDA_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.

          `IDA_BAD_DKY`   `dkyQS` or one of the vectors `dkyQS[i]` is NULL.

          `IDA_BAD_K`   `k` is not in the range $0, 1, ..., klast$.

          `IDA_BAD_T`   The time `t` is not in the allowed range.

F2003 Name `FIDAGetQuadSensDky`

Quadrature sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions `IDAGetQuadSens1` and `IDAGetQuadSensDky1`, defined as follows:

IDAGetQuadSens1

Call   `flag = IDAGetQuadSens1(ida_mem, &tret, is, yQS);`

Description   The function `IDAGetQuadSens1` returns the `is`-th sensitivity of quadratures after a successful return from `IDASolve`.

Arguments   `ida_mem` (`void *`) pointer to the memory previously allocated by `IDAInit`.

          `tret`   (`realtype`) the time reached by the solver (output).

          `is`   (`int`) specifies which sensitivity vector is to be returned ($0 \leq$ `is` $< N_s$).

          `yQS`   (`N_Vector`) the computed sensitivity-dependent quadrature vector. This vector must be allocated by the user.

Return value The return value `flag` of `IDAGetQuadSens1` is one of:

          `IDA_SUCCESS`   `IDAGetQuadSens1` was successful.

          `IDA_MEM_NULL`   `ida_mem` was NULL.

          `IDA_NO_SENS`   Forward sensitivity analysis was not initialized.

          `IDA_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.

          `IDA_BAD_IS`   The index `is` is not in the allowed range.

          `IDA_BAD_DKY`   `yQS` is NULL.

F2003 Name `FIDAGetQuadSens1`

IDAGetQuadSensDky1

Call   `flag = IDAGetQuadSensDky1(ida_mem, t, k, is, dkyQS);`

Description   The function `IDAGetQuadSensDky1` returns the `k`-th derivative of the `is`-th sensitivity solution vector after a successful return from `IDASolve`.

Arguments   ida_mem (void *) pointer to the memory previously allocated by IDAInit.

   t   (realtype) specifies the time at which sensitivity information is requested. The time t must fall within the interval defined by the last successful step taken by IDAS.

   k   (int) order of derivative. k must be in the range $0, 1, ..., klast$ where $klast$ is the method order of the last successful step.

   is   (int) specifies the sensitivity derivative vector to be returned ($0 \leq$ is $< N_s$).

   dkyQS   (N_Vector) the vector containing the derivative. The space for dkyQS must be allocated by the user.

Return value The return value flag of IDAGetQuadSensDky1 is one of:

   IDA_SUCCESS   IDAGetQuadDky1 succeeded.

   IDA_MEM_NULL   ida_mem was NULL.

   IDA_NO_SENS   Forward sensitivity analysis was not initialized.

   IDA_NO_QUADSENS Quadratures depending on the sensitivities were not activated.

   IDA_BAD_DKY   dkyQS is NULL.

   IDA_BAD_IS   The index is is not in the allowed range.

   IDA_BAD_K   k is not in the range $0, 1, ..., klast$.

   IDA_BAD_T   The time t is not in the allowed range.

F2003 Name FIDAGetQuadSensDky1

5.4.4   Optional inputs for sensitivity-dependent quadrature integration

IDAS provides the following optional input functions to control the integration of sensitivity-dependent quadrature equations.

IDASetQuadSensErrCon

Call   flag = IDASetQuadSensErrCon(ida_mem, errconQS)

Description The function IDASetQuadSensErrCon specifies whether or not the quadrature variables are to be used in the local error control mechanism. If they are, the user must specify the error tolerances for the quadrature variables by calling IDAQuadSensSStolerances, IDAQuadSensSVtolerances, or IDAQuadSensEEtolerances.

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

   errconQS (booleantype) specifies whether sensitivity quadrature variables are included (SUNTRUE) or not (SUNFALSE) in the error control mechanism.

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

   IDA_SUCCESS   The optional value has been successfully set.

   IDA_MEM_NULL   The ida_mem pointer is NULL.

   IDA_NO_SENS   Sensitivities were not activated.

   IDA_NO_QUADSENS Quadratures depending on the sensitivities were not activated.

Notes   By default, errconQS is set to SUNFALSE.

   It is illegal to call IDASetQuadSensErrCon before a call to IDAQuadSensInit.

F2003 Name FIDASetQuadSensErrCon

   If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

`IDAQuadSensSStolerances`

Call	`flag = IDAQuadSensSVtolerances(ida_mem, reltolQS, abstolQS);`
Description	The function `IDAQuadSensSStolerances` specifies scalar relative and absolute tolerances.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`reltolQS` (`realtype`) is the scalar relative error tolerance.
	`abstolQS` (`realtype*`) is a pointer to an array containing the `Ns` scalar absolute error tolerances.
Return value	The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is NULL.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FIDAQuadSensSStolerances`

`IDAQuadSensSVtolerances`

Call	`flag = IDAQuadSensSVtolerances(ida_mem, reltolQS, abstolQS);`
Description	The function `IDAQuadSensSVtolerances` specifies scalar relative and vector absolute tolerances.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`reltolQS` (`realtype`) is the scalar relative error tolerance.
	`abstolQS` (`N_Vector*`) is an array of `Ns` variables of type `N_Vector`. The `N_Vector` from `abstolS[is]` specifies the vector tolerances for `is`-th quadrature sensitivity.
Return value	The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_NO_QUAD`	Quadrature integration was not initialized.
`IDA_MEM_NULL`	The `ida_mem` pointer is NULL.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`IDA_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FIDAQuadSensSVtolerances`

`IDAQuadSensEEtolerances`

Call	`flag = IDAQuadSensEEtolerances(ida_mem);`
Description	The function `IDAQuadSensEEtolerances` specifies that the tolerances for the sensitivity-dependent quadratures should be estimated from those provided for the pure quadrature variables.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
Return value	The return value `flag` (of type `int`) is one of:

`IDA_SUCCESS`	The optional value has been successfully set.
`IDA_MEM_NULL`	The `ida_mem` pointer is NULL.
`IDA_NO_SENS`	Sensitivities were not activated.
`IDA_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.

Notes   When `IDAQuadSensEEtolerances` is used, before calling `IDASolve`, integration of pure quadratures must be initialized (see 4.7.1) and tolerances for pure quadratures must be also specified (see 4.7.4).

F2003 Name   `FIDAQuadSensEEtolerances`

5.4.5   Optional outputs for sensitivity-dependent quadrature integration

IDAS provides the following functions that can be used to obtain solver performance information related to quadrature integration.

`IDAGetQuadSensNumRhsEvals`

Call   `flag = IDAGetQuadSensNumRhsEvals(ida_mem, &nrhsQSevals);`

Description   The function `IDAGetQuadSensNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.

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

                `nrhsQSevals` (`long int`) number of calls made to the user's `rhsQS` function.

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

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

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

                `IDA_NO_QUADSENS` Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name   `FIDAGetQuadSensNumRhsEvals`

`IDAGetQuadSensNumErrTestFails`

Call   `flag = IDAGetQuadSensNumErrTestFails(ida_mem, &nQSetfails);`

Description   The function `IDAGetQuadSensNumErrTestFails` returns the number of local error test failures due to quadrature variables.

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

                `nQSetfails` (`long int`) number of error test failures due to quadrature variables.

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

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

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

                `IDA_NO_QUADSENS` Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name   `FIDAGetQuadSensNumErrTestFails`

`IDAGetQuadSensErrWeights`

Call   `flag = IDAGetQuadSensErrWeights(ida_mem, eQSweight);`

Description   The function `IDAGetQuadSensErrWeights` returns the quadrature error weights at the current time.

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

                `eQSweight` (`N_Vector *`) array of quadrature error weight vectors at the current time.

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

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

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

                `IDA_NO_QUADSENS` Sensitivity-dependent quadrature integration has not been initialized.

Notes   The user must allocate memory for `eQSweight`.

               If quadratures were not included in the error control mechanism (through a call to
               `IDASetQuadSensErrCon` with `errconQS=SUNTRUE`), `IDAGetQuadSensErrWeights` does
               not set the `eQSweight` vector.

F2003 Name `FIDAGetQuadSensErrWeights`

| `IDAGetQuadSensStats` |

Call   `flag = IDAGetQuadSensStats(ida_mem, &nrhsQSevals, &nQSetfails);`

Description   The function `IDAGetQuadSensStats` returns the IDAS integrator statistics as a group.

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

              `nrhsQSevals` (`long int`) number of calls to the user's `rhsQS` function.

              `nQSetfails` (`long int`) number of error test failures due to quadrature variables.

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

              `IDA_SUCCESS`   the optional output values have been successfully set.

              `IDA_MEM_NULL`   the `ida_mem` pointer is `NULL`.

              `IDA_NO_QUADSENS` Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name `FIDAGetQuadSensStats`

5.4.6   User-supplied function for sensitivity-dependent quadrature integration

For the integration of sensitivity-dependent quadrature equations, the user must provide a function
that defines the right-hand side of the sensitivity quadrature equations. For sensitivities of quadratures
(2.10) with integrands q, the appropriate right-hand side functions are given by $\bar{q}_i = (\partial q/\partial y)s_i + (\partial q/\partial \dot{y})\dot{s}_i + \partial q/\partial p_i$. This user function must be of type `IDAQuadSensRhsFn`, defined as follows:

| `IDAQuadSensRhsFn` |

Definition   `typedef int (*IDAQuadSensRhsFn)(int Ns, realtype t, N_Vector yy,`
                                           `N_Vector yp, N_Vector *yyS, N_Vector *ypS,`
                                           `N_Vector rrQ, N_Vector *rhsvalQS,`
                                           `void *user_data, N_Vector tmp1,`
                                           `N_Vector tmp2, N_Vector tmp3)`

Purpose   This function computes the sensitivity quadrature equation right-hand side for a given
              value of the independent variable t and state vector y.

Arguments   `Ns`   is the number of sensitivity vectors.

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

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

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

              `yyS`   is an array of `Ns` variables of type `N_Vector` containing the dependent sensitivity vectors s_i.

              `ypS`   is an array of `Ns` variables of type `N_Vector` containing the dependent sensitivity derivatives $\dot{s}_i$.

              `rrQ`   is the current value of the quadrature right-hand side q.

              `rhsvalQS`   contains the `Ns` output vectors.

              `user_data`   is the `user_data` pointer passed to `IDASetUserData`.

              `tmp1`
              `tmp2`

tmp3   are N_Vectors which can be used as temporary storage.

Return value   An IDAQuadSensRhsFn should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and IDA_QRHS_FAIL is returned).

Notes   Allocation of memory for rhsvalQS is automatically handled within IDAS.

Both yy and yp are of type N_Vector and both yyS and ypS are pointers to an array containing Ns vectors of type N_Vector. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their N_Vector arguments (see §9.3 and §9.4).

There is one situation in which recovery is not possible even if IDAQuadSensRhsFn function returns a recoverable error flag. That is when this occurs at the very first call to the IDAQuadSensRhsFn, in which case IDAS returns IDA_FIRST_QSRHS_ERR).

5.5   Note on using partial error control

For some problems, when sensitivities are excluded from the error control test, the behavior of IDAS may appear at first glance to be erroneous. One would expect that, in such cases, the sensitivity variables would not influence in any way the step size selection.

The short explanation of this behavior is that the step size selection implemented by the error control mechanism in IDAS is based on the magnitude of the correction calculated by the nonlinear solver. As mentioned in §5.2.1, even with partial error control selected in the call to IDASensInit, the sensitivity variables are included in the convergence tests of the nonlinear solver.

When using the simultaneous corrector method (§2.5), the nonlinear system that is solved at each step involves both the state and sensitivity equations. In this case, it is easy to see how the sensitivity variables may affect the convergence rate of the nonlinear solver and therefore the step size selection. The case of the staggered corrector approach is more subtle. The sensitivity variables at a given step are computed only once the solver for the nonlinear state equations has converged. However, if the nonlinear system corresponding to the sensitivity equations has convergence problems, IDAS will attempt to improve the initial guess by reducing the step size in order to provide a better prediction of the sensitivity variables. Moreover, even if there are no convergence failures in the solution of the sensitivity system, IDAS may trigger a call to the linear solver's setup routine which typically involves reevaluation of Jacobian information (Jacobian approximation in the case of IDADENSE and IDABAND, or preconditioner data in the case of the Krylov solvers). The new Jacobian information will be used by subsequent calls to the nonlinear solver for the state equations and, in this way, potentially affect the step size selection.

When using the simultaneous corrector method it is not possible to decide whether nonlinear solver convergence failures or calls to the linear solver setup routine have been triggered by convergence problems due to the state or the sensitivity equations. When using one of the staggered corrector methods, however, these situations can be identified by carefully monitoring the diagnostic information provided through optional outputs. If there are no convergence failures in the sensitivity nonlinear solver, and none of the calls to the linear solver setup routine were made by the sensitivity nonlinear solver, then the step size selection is not affected by the sensitivity variables.

Finally, the user must be warned that the effect of appending sensitivity equations to a given system of DAEs on the step size selection (through the mechanisms described above) is problem-dependent and can therefore lead to either an increase or decrease of the total number of steps that IDAS takes to complete the simulation. At first glance, one would expect that the impact of the sensitivity variables, if any, would be in the direction of increasing the step size and therefore reducing the total number of steps. The argument for this is that the presence of the sensitivity variables in the convergence test of the nonlinear solver can only lead to additional iterations (and therefore a smaller iteration error), or to additional calls to the linear solver setup routine (and therefore more up-to-date Jacobian

information), both of which will lead to larger steps being taken by IDAS. However, this is true only locally. Overall, a larger integration step taken at a given time may lead to step size reductions at later times, due to either nonlinear solver convergence failures or error test failures.

Chapter 6

Using IDAS for Adjoint Sensitivity Analysis

This chapter describes the use of IDAS to compute sensitivities of derived functions using adjoint sensitivity analysis. As mentioned before, the adjoint sensitivity module of IDAS provides the infrastructure for integrating backward in time any system of DAEs that depends on the solution of the original IVP, by providing various interfaces to the main IDAS integrator, as well as several supporting user-callable functions. For this reason, in the following sections we refer to the *backward problem* and not to the *adjoint problem* when discussing details relevant to the DAEs that are integrated backward in time. The backward problem can be the adjoint problem (2.20) or (2.25), and can be augmented with some quadrature differential equations.

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

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable functions and of the user-supplied functions that were not already described in Chapter 4.

6.1 A skeleton of the user's main program

The following is a skeleton of the user's main program as an application of IDAS. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapters 9, 10, 11, and 12 for the specific name of the function to be called or macro to be referenced.

Steps that are unchanged from the skeleton programs presented in §4.4, §5.1, and §5.4, are grayed out.

1. **Include necessary header files**

   The `idas.h` header file also defines additional types, constants, and function prototypes for the adjoint sensitivity module user-callable functions. In addition, the main program should include an NVECTOR implementation header file (for the particular implementation used) and, if a nonlinear solver requiring a linear solver (e.g., the default Newton iteration) will be used, the header file of the desired linear solver module.

2. **Initialize parallel or multi-threaded environment**

<div align="center">

Forward problem

</div>

3. **Set problem dimensions etc. for the forward problem**

4. **Set initial conditions for the forward problem**

5. **Create** IDAS **object for the forward problem**

6. **Initialize** IDAS **solver for the forward problem**

7. **Specify integration tolerances for forward problem**

8. **Set optional inputs for the forward problem**

9. **Create matrix object for the forward problem**

10. **Create linear solver object for the forward problem**

11. **Set linear solver optional inputs for the forward problem**

12. **Attach linear solver module for the forward problem**

13. **Create nonlinear solver module for the forward problem**

14. **Attach nonlinear solver module for the forward problem**

15. **Set nonlinear solver optional inputs for the forward problem**

16. **Initialize quadrature problem or problems for forward problems, using** `IDAQuadInit` **and/or** `IDAQuadSensInit`**.**

17. **Initialize forward sensitivity problem**

18. **Specify rootfinding**

19. **Allocate space for the adjoint computation**

    Call `IDAAdjInit()` to allocate memory for the combined forward-backward problem (see §6.2.1 for details). This call requires `Nd`, the number of steps between two consecutive checkpoints. `IDAAdjInit` also specifies the type of interpolation used (see §2.6.3).

20. **Integrate forward problem**

    Call `IDASolveF`, a wrapper for the IDAS main integration function `IDASolve`, either in `IDA_NORMAL` mode to the time `tout` or in `IDA_ONE_STEP` mode inside a loop (if intermediate solutions of the forward problem are desired (see §6.2.3)). The final value of `tret` is then the maximum allowable value for the endpoint T of the backward problem.

<div align="center">

Backward problem(s)

</div>

21. **Set problem dimensions etc. for the backward problem**

    This generally includes `NB`, the number of variables in the backward problem and possibly the local vector length `NBlocal`.

22. **Set initial values for the backward problem**

    Set the endpoint time `tB0` $= T$, and set the corresponding vectors `yB0` and `ypB0` at which the backward problem starts.

23. **Create the backward problem**

    Call `IDACreateB`, a wrapper for `IDACreate`, to create the IDAS memory block for the new backward problem. Unlike `IDACreate`, the function `IDACreateB` does not return a pointer to the newly created memory block (see §6.2.4). Instead, this pointer is attached to the internal adjoint memory block (created by `IDAAdjInit`) and returns an identifier called `which` that the user must later specify in any actions on the newly created backward problem.

24. **Allocate memory for the backward problem**

    Call `IDAInitB` (or `IDAInitBS`, when the backward problem depends on the forward sensitivities). The two functions are actually wrappers for `IDAInit` and allocate internal memory, specify problem data, and initialize IDAS at `tB0` for the backward problem (see §6.2.4).

25. **Specify integration tolerances for backward problem**

    Call `IDASStolerancesB(...)` or `IDASVtolerancesB(...)` to specify a scalar relative tolerance and scalar absolute tolerance, or a scalar relative tolerance and a vector of absolute tolerances, respectively. The functions are wrappers for `IDASStolerances(...)` and `IDASVtolerances(...)` but they require an extra argument `which`, the identifier of the backward problem returned by `IDACreateB`. See §6.2.5 for more information.

26. **Set optional inputs for the backward problem**

    Call `IDASet*B` functions to change from their default values any optional inputs that control the behavior of IDAS. Unlike their counterparts for the forward problem, these functions take an extra argument `which`, the identifier of the backward problem returned by `IDACreateB` (see §6.2.10).

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

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

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

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

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

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

    Note that it is not required to use the same linear solver module for both the forward and the backward problems; for example, the forward problem could be solved with the SUNLINSOL_DENSE linear solver module and the backward problem with SUNLINSOL_SPGMR linear solver module.

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

    Call `IDASet*B` functions to change optional inputs specific to the linear solver interface. See §6.2.10 for details.

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

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

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

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

    If using a non-default nonlinear solver for the backward problem, then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular SUNNONLINSOL implementation e.g., `NLSB = SUNNonlinSol_***(...);` where `***` is the name of the nonlinear solver (see Chapter 12 for details).

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

If using a non-default nonlinear solver for the backward problem, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling
`ier = IDASetNonlinearSolverB(idaode_mem, NLSB);` (see §6.2.7 for details).

33. **Initialize quadrature calculation**

    If additional quadrature equations must be evaluated, call `IDAQuadInitB` or `IDAQuadInitBS` (if quadrature depends also on the forward sensitivities) as shown in §6.2.12.1. These functions are wrappers around `IDAQuadInit` and can be used to initialize and allocate memory for quadrature integration. Optionally, call `IDASetQuad*B` functions to change from their default values optional inputs that control the integration of quadratures during the backward phase.

34. **Integrate backward problem**

    Call `IDASolveB`, a second wrapper around the IDAS main integration function `IDASolve`, to integrate the backward problem from `tB0` (see §6.2.9). This function can be called either in `IDA_NORMAL` or `IDA_ONE_STEP` mode. Typically, `IDASolveB` will be called in `IDA_NORMAL` mode with an end time equal to the initial time t_0 of the forward problem.

35. **Extract quadrature variables**

    If applicable, call `IDAGetQuadB`, a wrapper around `IDAGetQuad`, to extract the values of the quadrature variables at the time returned by the last call to `IDASolveB`. See §6.2.12.2.

36. **Deallocate memory**

    Upon completion of the backward integration, call all necessary deallocation functions. These include appropriate destructors for the vectors `y` and `yB`, a call to `IDAFree` to free the IDAS memory block for the forward problem. If one or more additional adjoint sensitivity analyses are to be done for this problem, a call to `IDAAdjFree` (see §6.2.1) may be made to free and deallocate the memory allocated for the backward problems, followed by a call to `IDAAdjInit`.

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

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

39. Finalize MPI, if used

The above user interface to the adjoint sensitivity module in IDAS was motivated by the desire to keep it as close as possible in look and feel to the one for DAE IVP integration. Note that if steps (21)-(35) are not present, a program with the above structure will have the same functionality as one described in §4.4 for integration of DAEs, albeit with some overhead due to the checkpointing scheme.

If there are multiple backward problems associated with the same forward problem, repeat steps (21)-(35) above for each successive backward problem. In the process, each call to `IDACreateB` creates a new value of the identifier `which`.

6.2   User-callable functions for adjoint sensitivity analysis

6.2.1   Adjoint sensitivity allocation and deallocation functions

After the setup phase for the forward problem, but before the call to `IDASolveF`, memory for the combined forward-backward problem must be allocated by a call to the function `IDAAdjInit`. The form of the call to this function is

IDAAdjInit

Call   `flag = IDAAdjInit(ida_mem, Nd, interpType);`

Description	The function `IDAAdjInit` updates IDAS memory block by allocating the internal memory needed for backward integration. Space is allocated for the $\mathtt{Nd} = N_d$ interpolation data points, and a linked list of checkpoints is initialized.
Arguments	`ida_mem` (`void *`) is the pointer to the IDAS memory block returned by a previous call to `IDACreate`.
	`Nd` (`long int`) is the number of integration steps between two consecutive checkpoints.
	`interpType` (`int`) specifies the type of interpolation used and can be `IDA_POLYNOMIAL` or `IDA_HERMITE`, indicating variable-degree polynomial and cubic Hermite interpolation, respectively (see §2.6.3).
Return value	The return value `flag` (of type `int`) is one of:
	`IDA_SUCCESS` `IDAAdjInit` was successful.
	`IDA_MEM_FAIL` A memory allocation request has failed.
	`IDA_MEM_NULL` `ida_mem` was NULL.
	`IDA_ILL_INPUT` One of the parameters was invalid: `Nd` was not positive or `interpType` is not one of the `IDA_POLYNOMIAL` or `IDA_HERMITE`.
Notes	The user must set `Nd` so that all data needed for interpolation of the forward problem solution between two checkpoints fits in memory. `IDAAdjInit` attempts to allocate space for (2`Nd`+3) variables of type `N_Vector`.
	If an error occurred, `IDAAdjInit` also sends a message to the error handler function.
F2003 Name	`FIDAAdjInit`

`IDAAdjReInit`

Call	`flag = IDAAdjReInit(ida_mem);`
Description	The function `IDAAdjReInit` reinitializes the IDAS memory block for ASA, assuming that the number of steps between check points and the type of interpolation remain unchanged.
Arguments	`ida_mem` (`void *`) is the pointer to the IDAS memory block returned by a previous call to `IDACreate`.
Return value	The return value `flag` (of type `int`) is one of:
	`IDA_SUCCESS` `IDAAdjReInit` was successful.
	`IDA_MEM_NULL` `ida_mem` was NULL.
	`IDA_NO_ADJ` The function `IDAAdjInit` was not previously called.
Notes	The list of check points (and associated memory) is deleted.
	The list of backward problems is kept. However, new backward problems can be added to this list by calling `IDACreateB`. If a new list of backward problems is also needed, then free the adjoint memory (by calling `IDAAdjFree`) and reinitialize ASA with `IDAAdjInit`.
	The IDAS memory for the forward and backward problems can be reinitialized separately by calling `IDAReInit` and `IDAReInitB`, respectively.
F2003 Name	`FIDAAdjReInit`

`IDAAdjFree`

Call	`IDAAdjFree(ida_mem);`
Description	The function `IDAAdjFree` frees the memory related to backward integration allocated by a previous call to `IDAAdjInit`.

Arguments   The only argument is the IDAS memory block pointer returned by a previous call to
            `IDACreate`.

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

Notes   This function frees all memory allocated by `IDAAdjInit`. This includes workspace
            memory, the linked list of checkpoints, memory for the interpolation data, as well as
            the IDAS memory for the backward integration phase.

            Unless one or more further calls to `IDAAdjInit` are to be made, `IDAAdjFree` should not
            be called by the user, as it is invoked automatically by `IDAFree`.

F2003 Name `FIDAAdjFree`

6.2.2   Adjoint sensitivity optional input

At any time during the integration of the forward problem, the user can disable the checkpointing of
the forward sensitivities by calling the following function:

`IDAAdjSetNoSensi`

Call   `flag = IDAAdjSetNoSensi(ida_mem);`

Description The function `IDAAdjSetNoSensi` instructs `IDASolveF` not to save checkpointing data
            for forward sensitivities any more.

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

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

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

            `IDA_MEM_NULL` The `ida_mem` was `NULL`.

            `IDA_NO_ADJ`   The function `IDAAdjInit` has not been previously called.

F2003 Name `FIDAAdjSetNoSensi`

6.2.3   Forward integration function

The function `IDASolveF` is very similar to the IDAS function `IDASolve` (see §4.5.7) in that it integrates
the solution of the forward problem and returns the solution $(y, \dot{y})$. At the same time, however,
`IDASolveF` stores checkpoint data every `Nd` integration steps. `IDASolveF` can be called repeatedly
by the user. Note that `IDASolveF` is used only for the forward integration pass within an Adjoint
Sensitivity Analysis. It is not for use in Forward Sensitivity Analysis; for that, see Chapter 5. The
call to this function has the form

`IDASolveF`

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

Description The function `IDASolveF` integrates the forward problem over an interval in t and saves
            checkpointing data.

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

            `tout`   (`realtype`) the next time at which a computed solution is desired.

            `tret`   (`realtype`) the time reached by the solver (output).

            `yret`   (`N_Vector`) the computed solution vector y.

            `ypret`   (`N_Vector`) the computed solution vector $\dot{y}$.

            `itask`   (`int`) a flag indicating the job of the solver for the next step. The `IDA_NORMAL`
                      task is to have the solver take internal steps until it has reached or just passed
                      the user-specified `tout` parameter. The solver then interpolates in order to
                      return an approximate value of $y(\texttt{tout})$ and $\dot{y}(\texttt{tout})$. The `IDA_ONE_STEP` option
                      tells the solver to take just one internal step and return the solution at the
                      point reached by that step.

ncheck (`int`) the number of (internal) checkpoints stored so far.

Return value On return, `IDASolveF` returns vectors `yret`, `ypret` and a corresponding independent variable value $t = $ `tret`, such that `yret` is the computed value of $y(t)$ and `ypret` the value of $\dot{y}(t)$. Additionally, it returns in `ncheck` the number of internal checkpoints saved; the total number of checkpoint intervals is `ncheck`+1. The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.7.

`IDA_SUCCESS`	`IDASolveF` succeeded.
`IDA_TSTOP_RETURN`	`IDASolveF` succeeded by reaching the optional stopping point.
`IDA_ROOT_RETURN`	`IDASolveF` succeeded and found one or more roots. In this case, `tret` is the location of the root. If `nrtfn` > 1, call `IDAGetRootInfo` to see which g_i were found to have a root.
`IDA_NO_MALLOC`	The function `IDAInit` has not been previously called.
`IDA_ILL_INPUT`	One of the inputs to `IDASolveF` is illegal.
`IDA_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tout`.
`IDA_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`IDA_ERR_FAILURE`	Error test failures occurred too many times during one internal time step or occurred with $|h| = h_{min}$.
`IDA_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step or occurred with $|h| = h_{min}$.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_MEM_FAIL`	A memory allocation request has failed (in an attempt to allocate space for a new checkpoint).

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

At this time, `IDASolveF` stores checkpoint information in memory only. Future versions will provide for a safeguard option of dumping checkpoint data into a temporary file as needed. The data stored at each checkpoint is basically a snapshot of the IDAS internal memory block and contains enough information to restart the integration from that time and to proceed with the same step size and method order sequence as during the forward integration.

In addition, `IDASolveF` also stores interpolation data between consecutive checkpoints so that, at the end of this first forward integration phase, interpolation information is already available from the last checkpoint forward. In particular, if no checkpoints were necessary, there is no need for the second forward integration phase.

It is illegal to change the integration tolerances between consecutive calls to `IDASolveF`, as this information is not captured in the checkpoint data.

F2003 Name `FIDASolveF`

6.2.4 Backward problem initialization functions

The functions `IDACreateB` and `IDAInitB` (or `IDAInitBS`) must be called in the order listed. They instantiate an IDAS solver object, provide problem and solution specifications, and allocate internal memory for the backward problem.

IDACreateB

Call	`flag = IDACreateB(ida_mem, &which);`
Description	The function `IDACreateB` instantiates an IDAS solver object for the backward problem.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`which` (`int`) contains the identifier assigned by IDAS for the newly created backward problem. Any call to `IDA*B` functions requires such an identifier.
Return value	The return `flag` (of type `int`) is one of:
	`IDA_SUCCESS` The call to `IDACreateB` was successful.
	`IDA_MEM_NULL` The `ida_mem` was NULL.
	`IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
	`IDA_MEM_FAIL` A memory allocation request has failed.
F2003 Name	`FIDACreateB`

There are two initialization functions for the backward problem – one for the case when the backward problem does not depend on the forward sensitivities, and one for the case when it does. These two functions are described next.

The function `IDAInitB` initializes the backward problem when it does not depend on the forward sensitivities. It is essentially wrapper for `IDAInit` with some particularization for backward integration, as described below.

IDAInitB

Call	`flag = IDAInitB(ida_mem, which, resB, tB0, yB0, ypB0);`
Description	The function `IDAInitB` provides problem specification, allocates internal memory, and initializes the backward problem.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
	`which` (`int`) represents the identifier of the backward problem.
	`resB` (`IDAResFnB`) is the C function which computes fB, the residual of the backward DAE problem. This function has the form `resB(t, y, yp, yB, ypB, resvalB, user_dataB)` (for full details see §6.3.1).
	`tB0` (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem, normally equal to the endpoint of the forward integration.
	`yB0` (`N_Vector`) is the initial value (at $t = $ `tB0`) of the backward solution.
	`ypB0` (`N_Vector`) is the initial derivative value (at $t = $ `tB0`) of the backward solution.
Return value	The return `flag` (of type `int`) will be one of the following:
	`IDA_SUCCESS` The call to `IDAInitB` was successful.
	`IDA_NO_MALLOC` The function `IDAInit` has not been previously called.
	`IDA_MEM_NULL` The `ida_mem` was NULL.
	`IDA_NO_ADJ` The function `IDAAdjInit` has not been previously called.
	`IDA_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
	`IDA_ILL_INPUT` The parameter `which` represented an invalid identifier, or one of `yB0`, `ypB0`, `resB` was NULL.
Notes	The memory allocated by `IDAInitB` is deallocated by the function `IDAAdjFree`.
F2003 Name	`FIDAInitB`

For the case when backward problem also depends on the forward sensitivities, user must call `IDAInitBS` instead of `IDAInitB`. Only the third argument of each function differs between these functions.

IDAInitBS

Call   `flag = IDAInitBS(ida_mem, which, resBS, tB0, yB0, ypB0);`

Description   The function `IDAInitBS` provides problem specification, allocates internal memory, and initializes the backward problem.

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

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

           `resBS`   (`IDAResFnBS`) is the C function which computes fB, the residual or the backward DAE problem. This function has the form `resBS(t, y, yp, yS, ypS, yB, ypB, resvalB, user_dataB)` (for full details see §6.3.2).

           `tB0`   (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem.

           `yB0`   (`N_Vector`) is the initial value (at $t = $ `tB0`) of the backward solution.

           `ypB0`   (`N_Vector`) is the initial derivative value (at $t = $ `tB0`) of the backward solution.

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

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

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

         `IDA_MEM_NULL`   The `ida_mem` was NULL.

         `IDA_NO_ADJ`   The function `IDAAdjInit` has not been previously called.

         `IDA_BAD_TB0`   The final time `tB0` was outside the interval over which the forward problem was solved.

         `IDA_ILL_INPUT`   The parameter `which` represented an invalid identifier, or one of `yB0`, `ypB0`, `resB` was NULL, or sensitivities were not active during the forward integration.

Notes   The memory allocated by `IDAInitBS` is deallocated by the function `IDAAdjFree`.

F2003 Name   `FIDAInitBS`

The function `IDAReInitB` reinitializes IDAS for the solution of a series of backward problems, each identified by a value of the parameter `which`. `IDAReInitB` is essentially a wrapper for `IDAReInit`, and so all details given for `IDAReInit` in §4.5.11 apply here. Also, `IDAReInitB` can be called to reinitialize a backward problem even if it has been initialized with the sensitivity-dependent version `IDAInitBS`. Before calling `IDAReInitB` for a new backward problem, call any desired solution extraction functions `IDAGet**` associated with the previous backward problem. The call to the `IDAReInitB` function has the form

---

IDAReInitB

Call   `flag = IDAReInitB(ida_mem, which, tB0, yB0, ypB0)`

Description   The function `IDAReInitB` reinitializes an IDAS backward problem.

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

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

           `tB0`   (`realtype`) specifies the endpoint T where final conditions are provided for the backward problem.

           `yB0`   (`N_Vector`) is the initial value (at $t = $ `tB0`) of the backward solution.

           `ypB0`   (`N_Vector`) is the initial derivative value (at $t = $ `tB0`) of the backward solution.

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

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

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

         `IDA_MEM_NULL`   The `ida_mem` memory block pointer was NULL.

         `IDA_NO_ADJ`   The function `IDAAdjInit` has not been previously called.

IDA_BAD_TB0　　The final time `tB0` is outside the interval over which the forward problem was solved.

IDA_ILL_INPUT　The parameter `which` represented an invalid identifier, or one of `yB0`, `ypB0` was NULL.

F2003 Name　`FIDAReInitB`

6.2.5　Tolerance specification functions for backward problem

One of the following two functions must be called to specify the integration tolerances for the backward problem. Note that this call must be made after the call to `IDAInitB` or `IDAInitBS`.

IDASStolerancesB

Call　　　　　`flag = IDASStolerances(ida_mem, which, reltolB, abstolB);`

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

Arguments　`ida_mem` (`void *`) pointer to the IDAS memory block returned by `IDACreate`.
　　　　　　`which`　(`int`) represents the identifier of the backward problem.
　　　　　　`reltolB` (`realtype`) is the scalar relative error tolerance.
　　　　　　`abstolB` (`realtype`) is the scalar absolute error tolerance.

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

IDA_SUCCESS　　The call to `IDASStolerancesB` was successful.

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

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

IDA_NO_ADJ　　The function `IDAAdjInit` has not been previously called.

IDA_ILL_INPUT　One of the input tolerances was negative.

F2003 Name　`FIDASStolerancesB`

IDASVtolerancesB

Call　　　　　`flag = IDASVtolerancesB(ida_mem, which, reltolB, abstolB);`

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

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

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

IDA_SUCCESS　　The call to `IDASVtolerancesB` was successful.

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

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

IDA_NO_ADJ　　The function `IDAAdjInit` has not been previously called.

IDA_ILL_INPUT　The relative error tolerance was negative or the absolute tolerance had a negative component.

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

F2003 Name　`FIDASVtolerancesB`

6.2.6 Linear solver initialization functions for backward problem

All IDAS linear solver modules available for forward problems are available for the backward problem. They should be created as for the forward problem then attached to the memory structure for the backward problem using the following function.

IDASetLinearSolverB

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

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

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

              `which`   (`int`) represents the identifier of the backward problem returned by `IDACreateB`.

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

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

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

       `IDALS_SUCCESS` The IDALS initialization was successful.

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

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

       `IDALS_MEM_FAIL` A memory allocation request failed.

       `IDALS_NO_ADJ` The function `IDAAdjInit` has not been previously called.

       `IDALS_ILL_INPUT` The parameter `which` represented an invalid identifier.

Notes   If `LS` is a matrix-based linear solver, then the template Jacobian matrix `A` will be used in the solve process, so if additional storage is required within the SUNMATRIX object (e.g. for factorization of a banded matrix), ensure that the input object is allocated with sufficient size (see the documentation of the particular SUNMATRIX type in Chapter 10 for further information).

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

F2003 Name   `FIDASetLinearSolverB`

6.2.7 Nonlinear solver initialization functions for backward problem

As with the forward problem IDAS uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §12.3) by default.

To specify a different nonlinear solver in IDAS for the backward problem, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to IDAS by calling `IDASetNonlinearSolverB`, as documented below.

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

IDASetNonlinearSolverB

Call	`flag = IDASetNonlinearSolverB(ida_mem, which, NLS);`

Description The function `IDASetNonLinearSolverB` attaches a SUNNONLINSOL object (`NLS`) to IDAS for the solution of the backward problem.

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

`which` (`int`) represents the identifier of the backward problem returned by `IDACreateB`.

`NLS` (`SUNNonlinearSolver`) SUNNONLINSOL object to use for solving nonlinear systems for the backward problem.

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`.

`IDALS_NO_ADJ` The function `CVAdjInit` has not been previously called.

`IDA_ILL_INPUT` The parameter `which` represented an invalid identifier or the SUNNON-LINSOL 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 `FIDASetNonlinearSolverB`

6.2.8 Initial condition calculation functions for backward problem

IDAS provides support for calculation of consistent initial conditions for certain backward index-one problems of semi-implicit form through the functions `IDACalcICB` and `IDACalcICBS`. Calling them is optional. It is only necessary when the initial conditions do not satisfy the adjoint system.

The above functions provide the same functionality for backward problems as `IDACalcIC` with parameter `icopt` = `IDA_YA_YDP_INIT` provides for forward problems (see §4.5.5): compute the algebraic components of yB and differential components of $\dot{y}B$, given the differential components of yB. They require that the `IDASetIdB` was previously called to specify the differential and algebraic components.

Both functions require forward solutions at the final time `tB0`. `IDACalcICBS` also needs forward sensitivities at the final time `tB0`.

IDACalcICB

Call	`flag = IDACalcICB(ida_mem, which, tBout1, N_Vector yfin, N_Vector ypfin);`

Description The function `IDACalcICB` corrects the initial values `yB0` and `ypB0` at time `tB0` for the backward problem.

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

`which` (`int`) is the identifier of the backward problem.

`tBout1` (`realtype`) is the first value of t at which a solution will be requested (from `IDASolveB`). This value is needed here only to determine the direction of integration and rough scale in the independent variable t.

`yfin` (`N_Vector`) the forward solution at the final time `tB0`.

`ypfin` (`N_Vector`) the forward solution derivative at the final time `tB0`.

Return value The return value `flag` (of type `int`) can be any that is returned by `IDACalcIC` (see §4.5.5). However `IDACalcICB` can also return one of the following:

`IDA_NO_ADJ` `IDAAdjInit` has not been previously called.

`IDA_ILL_INPUT` Parameter `which` represented an invalid identifier.

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

              Note that `IDACalcICB` will correct the values of $yB(tB_0)$ and $\dot{y}B(tB_0)$ which were specified in the previous call to `IDAInitB` or `IDAReInitB`. To obtain the corrected values, call `IDAGetconsistentICB` (see §6.2.11.2).

F2003 Name   `FIDACalcICB`

    In the case where the backward problem also depends on the forward sensitivities, user must call the following function to correct the initial conditions:

IDACalcICBS

Call   `flag = IDACalcICBS(ida_mem, which, tBout1, N_Vector yfin, N_Vector ypfin,`
                                `N_Vector ySfin, N_Vector ypSfin);`

Description   The function `IDACalcICBS` corrects the initial values `yB0` and `ypB0` at time `tB0` for the backward problem.

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

           `which`   (`int`) is the identifier of the backward problem.

           `tBout1`   (`realtype`) is the first value of t at which a solution will be requested (from `IDASolveB`).This value is needed here only to determine the direction of integration and rough scale in the independent variable t.

           `yfin`   (`N_Vector`) the forward solution at the final time `tB0`.

           `ypfin`   (`N_Vector`) the forward solution derivative at the final time `tB0`.

           `ySfin`   (`N_Vector *`) a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution at the final time `tB0`.

           `ypSfin`   (`N_Vector *`) a pointer to an array of `Ns` vectors containing the derivatives of the forward solution sensitivities at the final time `tB0`.

Return value The return value `flag` (of type `int`) can be any that is returned by `IDACalcIC` (see §4.5.5). However `IDACalcICBS` can also return one of the following:

           `IDA_NO_ADJ`   `IDAAdjInit` has not been previously called.

           `IDA_ILL_INPUT` Parameter `which` represented an invalid identifier, sensitivities were not active during forward integration, or `IDAInitBS` (or `IDAReInitBS`) has not been previously called.

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

              Note that `IDACalcICBS` will correct the values of $yB(tB_0)$ and $\dot{y}B(tB_0)$ which were specified in the previous call to `IDAInitBS` or `IDAReInitBS`. To obtain the corrected values, call `IDAGetConsistentICB` (see §6.2.11.2).

F2003 Name   `FIDACalcICBS`

6.2.9   Backward integration function

The function `IDASolveB` performs the integration of the backward problem. It is essentially a wrapper for the IDAS main integration function `IDASolve` and, in the case in which checkpoints were needed, it evolves the solution of the backward problem through a sequence of forward-backward integration pairs between consecutive checkpoints. In each pair, the first run integrates the original IVP forward in time and stores interpolation data; the second run integrates the backward problem backward in time and performs the required interpolation to provide the solution of the IVP to the backward problem.

    The function `IDASolveB` does not return the solution `yB` itself. To obtain that, call the function `IDAGetB`, which is also described below.

The `IDASolveB` function does not support rootfinding, unlike `IDASoveF`, which supports the finding of roots of functions of $(t, y, \dot{y})$. If rootfinding was performed by `IDASolveF`, then for the sake of efficiency, it should be disabled for `IDASolveB` by first calling `IDARootInit` with `nrtfn = 0`.

The call to `IDASolveB` has the form

`IDASolveB`

Call	`flag = IDASolveB(ida_mem, tBout, itaskB);`
Description	The function `IDASolveB` integrates the backward DAE problem.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory returned by `IDACreate`.
	`tBout` (`realtype`) the next time at which a computed solution is desired.
	`itaskB` (`int`) a flag indicating the job of the solver for the next step. The `IDA_NORMAL` task is to have the solver take internal steps until it has reached or just passed the user-specified value `tBout`. The solver then interpolates in order to return an approximate value of $yB(\texttt{tBout})$. The `IDA_ONE_STEP` option tells the solver to take just one internal step in the direction of `tBout` and return.
Return value	The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.7.

`IDA_SUCCESS`	`IDASolveB` succeeded.
`IDA_MEM_NULL`	The `ida_mem` was NULL.
`IDA_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDA_NO_BCK`	No backward problem has been added to the list of backward problems by a call to `IDACreateB`
`IDA_NO_FWD`	The function `IDASolveF` has not been previously called.
`IDA_ILL_INPUT`	One of the inputs to `IDASolveB` is illegal.
`IDA_BAD_ITASK`	The `itaskB` argument has an illegal value.
`IDA_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tBout`.
`IDA_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`IDA_ERR_FAILURE`	Error test failures occurred too many times during one internal time step.
`IDA_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step.
`IDA_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`IDA_SOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`IDA_BCKMEM_NULL`	The IDAS memory for the backward problem was not created with a call to `IDACreateB`.
`IDA_BAD_TBOUT`	The desired output time `tBout` is outside the interval over which the forward problem was solved.
`IDA_REIFWD_FAIL`	Reinitialization of the forward problem failed at the first checkpoint (corresponding to the initial time of the forward problem).
`IDA_FWD_FAIL`	An error occurred during the integration of the forward problem.

Notes	All failure return values are negative and therefore a test `flag< 0` will trap all `IDASolveB` failures.
	In the case of multiple checkpoints and multiple backward problems, a given call to `IDASolveB` in `IDA_ONE_STEP` mode may not advance every problem one step, depending on the relative locations of the current times reached. But repeated calls will eventually advance all problems to `tBout`.
F2003 Name	`FIDASolveB`

To obtain the solution `yB` to the backward problem, call the function `IDAGetB` as follows:

IDAGetB

Call   `flag = IDAGetB(ida_mem, which, &tret, yB, ypB);`

Description   The function `IDAGetB` provides the solution `yB` of the backward DAE problem.

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

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

              `tret`   (`realtype`) the time reached by the solver (output).

              `yB`   (`N_Vector`) the backward solution at time `tret`.

              `ypB`   (`N_Vector`) the backward solution derivative at time `tret`.

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

              `IDA_SUCCESS`   `IDAGetB` was successful.

              `IDA_MEM_NULL`   `ida_mem` is NULL.

              `IDA_NO_ADJ`   The function `IDAAdjInit` has not been previously called.

              `IDA_ILL_INPUT` The parameter `which` is an invalid identifier.

Notes   The user must allocate space for `yB` and `ypB`.

              To obtain the solution associated with a given backward problem at some other time
              within the last integration step, first obtain a pointer to the proper IDAS memory struc-
              ture by calling `IDAGetAdjIDABmem` and then use it to call `IDAGetDky`.

F2003 Name   `FIDAGetB`

6.2.10   Optional input functions for the backward problem

As for the forward problem there are numerous optional input parameters that control the behavior
of the IDAS solver for the backward problem. IDAS provides functions that can be used to change
these optional input parameters from their default values which are then described in detail in the
remainder of this section, beginning with those for the main IDAS solver and continuing with those
for the linear solver interfaces. For the most casual use of IDAS, the reader can skip to §6.3.

   We note that, on an error return, all of the optional input functions 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***B` function can be made from the user's calling program at any time
and, if successful, takes effect immediately.

6.2.10.1   Main solver optional input functions

The adjoint module in IDAS provides wrappers for most of the optional input functions defined in
§4.5.8.1. The only difference is that the user must specify the identifier `which` of the backward
problem within the list managed by IDAS.

   The optional input functions defined for the backward problem are:

```
flag = IDASetUserDataB(ida_mem, which, user_dataB);
flag = IDASetMaxOrdB(ida_mem, which, maxordB);
flag = IDASetMaxNumStepsB(ida_mem, which, mxstepsB);
flag = IDASetInitStepB(ida_mem, which, hinB)
flag = IDASetMaxStepB(ida_mem, which, hmaxB);
flag = IDASetSuppressAlgB(ida_mem, which, suppressalgB);
flag = IDASetIdB(ida_mem, which, idB);
flag = IDASetConstraintsB(ida_mem, which, constraintsB);
```

Their return value `flag` (of type `int`) can have any of the return values of their counterparts, but it
can also be `IDA_NO_ADJ` if `IDAAdjInit` has not been called, or `IDA_ILL_INPUT` if `which` was an invalid
identifier.

6.2.10.2 Linear solver interface optional input functions

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

| `IDASetJacFnB` |

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

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

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

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

`jacB` (IDALsJacFnB) user-defined Jacobian approximation function.

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

IDALS_SUCCESS `IDASetJacFnB` succeeded.

IDALS_MEM_NULL The `ida_mem` was NULL.

IDALS_NO_ADJ The function `IDAAdjInit` has not been previously called.

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

IDALS_ILL_INPUT The parameter `which` represented an invalid identifier.

Notes The function type `IDALsJacFnB` is described in §6.3.5.

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

F2003 Name `FIDASetJacFnB`

| `IDASetJacFnBS` |

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

Description The function `IDASetJacFnBS` specifies the Jacobian approximation function to be used for the backward problem in the case where the backward problem depends on the forward sensitivities.

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

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

`jacBS` (IDALJacFnBS) user-defined Jacobian approximation function.

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

IDALS_SUCCESS `IDASetJacFnBS` succeeded.

IDALS_MEM_NULL The `ida_mem` was NULL.

IDALS_NO_ADJ The function `IDAAdjInit` has not been previously called.

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

IDALS_ILL_INPUT The parameter `which` represented an invalid identifier.

Notes The function type `IDALsJacFnBS` is described in §6.3.5.

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

F2003 Name `FIDASetJacFnBS`

The function `IDASetLinearSolutionScalingB` can be used to enable or disable solution scaling when using a matrix-based linear solver.

`IDASetLinearSolutionScalingB`

Call   `flag = IDASetLinearSolutionScaling(ida_mem, which, onoffB);`

Description   The function `SetLinearSolutionScalingB` enables or disables scaling the linear system solution to account for a change in α in the linear system in the backward problem. For more details see §11.4.1.

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

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

           `onoffB`   (`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   By default scaling is enabled with matrix-based linear solvers when using BDF methods.

F2003 Name   `FIDASetLinearSolutionScalingB`

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

`IDASetJacTimesB`

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

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

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

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

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

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

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

           `IDALS_SUCCESS`   The optional value has been successfully set.

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

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

           `IDALS_NO_ADJ`   The function `IDAAdjInit` has not been previously called.

           `IDALS_ILL_INPUT`   The parameter `which` represented an invalid identifier.

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

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

F2003 Name   `FIDASetJacTimesB`

IDASetJacTimesBS

Call	`flag = IDASetJacTimesBS(ida_mem, which, jsetupBS, jtimesBS);`
Description	The function `IDASetJacTimesBS` specifies the Jacobian-vector product setup and evaluation functions to be used, in the case where the backward problem depends on the forward sensitivities.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`which` (`int`) the identifier of the backward problem.
	`jtsetupBS` (`IDALsJacTimesSetupFnBS`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.
	`jtimesBS` (`IDALsJacTimesVecFnBS`) user-defined Jacobian-vector product function.
Return value	The return value `flag` (of type `int`) is one of:

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

Notes	The function types `IDALsJacTimesVecFnBS` and `IDALsJacTimesSetupFnBS` are described in §6.3.6.
	The previous routine `IDASpilsSetJacTimesBS` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

F2003 Name `FIDASetJacTimesBS`

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

IDASetIncrementFactorB

Call	`flag = IDASetIncrementFactorB(ida_mem, which, dqincfacB);`
Description	The function `IDASetIncrementFactorB` specifies the factor in the increments used in the difference quotient approximations to matrix-vector products for the backward problem.
	This routine can be used in both the cases where the backward problem does and does not depend on the forward sensitvities.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`which` (`int`) the identifier of the backward problem.
	`dqincfacB` (`realtype`) difference quotient approximation factor.
Return value	The return value `flag` (of type `int`) is one of

`IDALS_SUCCESS`	The optional value has been successfully set.
`IDALS_MEM_NULL`	The `ida_mem` pointer is `NULL`.
`IDALS_LMEM_NULL`	The IDALS linear solver has not been initialized.
`IDALS_NO_ADJ`	The function `IDAAdjInit` has not been previously called.
`IDALS_ILL_INPUT`	The value of `eplifacB` is negative.
`IDALS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes	The default value is 1.0.
	The previous routine `IDASpilsSetIncrementFactorB` is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

F2003 Name `FIDASetIncrementFactorB`

Additionally, When using the internal difference quotient for the backward problem, the user may also optionally supply an alternative residual function for use in the Jacobian-vector product approximation by calling `IDASetJacTimesResFnB`. The alternative residual side function should compute a suitable (and differentiable) approximation to the residual function provided to `IDAInitB` or `IDAInitBS`. For example, as done in [28] for the forward integration of an ODE in explicit form without sensitivity analysis, the alternative function may use lagged values when evaluating a nonlinearity in the right-hand side to avoid differencing a potentially non-differentiable factor.

`IDASetJacTimesResFnB`

Call	`flag = IDASetJacTimesResFnB(ida_mem, which, jtimesResFn);`
Description	The function `IDASetJacTimesResFnB` specifies an alternative DAE residual function for use in the internal Jacobian-vector product difference quotient approximation for the backward problem.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`which` (`int`) the identifier of the backward problem.
	`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_NO_ADJ` The function `IDAAdjInit` has not been previously called.
	`IDALS_ILL_INPUT` The parameter `which` represented an invalid identifier or 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 `IDASetLinearSolverB`.

F2003 Name `FIDASetJacTimesResFnB`

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

`IDASetPreconditionerB`

Call	`flag = IDASetPreconditionerB(ida_mem, which, psetupB, psolveB);`
Description	The function `IDASetPrecSolveFnB` specifies the preconditioner setup and solve functions for the backward integration.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block.
	`which` (`int`) the identifier of the backward problem.
	`psetupB` (`IDALsPrecSetupFnB`) user-defined preconditioner setup function.
	`psolveB` (`IDALsPrecSolveFnB`) user-defined preconditioner solve function.
Return value	The return value `flag` (of type `int`) is one of:
	`IDALS_SUCCESS` The optional value has been successfully set.
	`IDALS_MEM_NULL` The `ida_mem` memory block pointer was NULL.

IDALS_LMEM_NULL The IDALS linear solver has not been initialized.

IDALS_NO_ADJ   The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT   The parameter which represented an invalid identifier.

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

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

F2003 Name FIDASetPreconditionerB

IDASetPreconditionerBS

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

Description   The function IDASetPrecSolveFnBS specifies the preconditioner setup and solve functions for the backward integration, in the case where the backward problem depends on the forward sensitivities.

Arguments   ida_mem   (void *) pointer to the IDAS memory block.
               which   (int) the identifier of the backward problem.
               psetupBS (IDALsPrecSetupFnBS) user-defined preconditioner setup function.
               psolveBS (IDALsPrecSolveFnBS) user-defined preconditioner solve function.

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

IDALS_SUCCESS   The optional value has been successfully set.

IDALS_MEM_NULL   The ida_mem memory block pointer was NULL.

IDALS_LMEM_NULL   The IDALS linear solver has not been initialized.

IDALS_NO_ADJ   The function IDAAdjInit has not been previously called.

IDALS_ILL_INPUT   The parameter which represented an invalid identifier.

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

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

F2003 Name FIDASetPreconditionerBS

IDASetEpsLinB

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

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

Arguments   ida_mem (void *) pointer to the IDAS memory block.
               which   (int) the identifier of the backward problem.
               eplifacB (realtype) linear convergence safety factor ($>= 0.0$).

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

IDALS_SUCCESS   The optional value has been successfully set.

IDALS_MEM_NULL   The ida_mem pointer is NULL.

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

Notes   The default value is 0.05.

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

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

F2003 Name   `FIDASetEpsLinB`

IDASetLSNormFactorB

Call   `flag = IDASetLSNormFactorB(ida_mem, which, nrmfac);`

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

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

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

              `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

	IDALS_SUCCESS	The optional value has been successfully set.
	IDALS_MEM_NULL	The `ida_mem` pointer is `NULL`.
	IDALS_LMEM_NULL	The IDALS linear solver has not been initialized.
	IDALS_NO_ADJ	The function `IDAAdjInit` has not been previously called.
	IDALS_ILL_INPUT	The value of `eplifacB` is negative.
	IDALS_ILL_INPUT	The parameter `which` represented an invalid identifier.

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

Prior to the introduction of `N_VGetLength` in SUNDIALS v5.0.0 (IDAS v4.0.0) the value of `nrmfac` was computed using the vector dot product i.e., the `nrmfac < 0` case.

F2003 Name   `FIDASetLSNormFactorB`

6.2.11   Optional output functions for the backward problem

6.2.11.1   Main solver optional output functions

The user of the adjoint module in IDAS has access to any of the optional output functions described in §4.5.10, both for the main solver and for the linear solver modules. The first argument of these `IDAGet*` and `IDA*Get*` functions is the pointer to the IDAS memory block for the backward problem. In order to call any of these functions, the user must first call the following function to obtain this pointer:

IDAGetAdjIDABmem

Call	`ida_memB = IDAGetAdjIDABmem(ida_mem, which);`
Description	The function `IDAGetAdjIDABmem` returns a pointer to the IDAS memory block for the backward problem.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
	`which` (`int`) the identifier of the backward problem.
Return value	The return value, `ida_memB` (of type `void *`), is a pointer to the IDAS memory for the backward problem.
Notes	The user should not modify `ida_memB` in any way.
	Optional output calls should pass `ida_memB` as the first argument; thus, for example, to get the number of integration steps: `flag = IDAGetNumSteps(idas_memB,&nsteps)`.
F2003 Name	`FIDAGetAdjIDABmem`

To get values of the *forward* solution during a backward integration, use the following function. The input value of `t` would typically be equal to that at which the backward solution has just been obtained with `IDAGetB`. In any case, it must be within the last checkpoint interval used by `IDASolveB`.

IDAGetAdjY

Call	`flag = IDAGetAdjY(ida_mem, t, y, yp);`
Description	The function `IDAGetAdjY` returns the interpolated value of the forward solution y and its derivative during a backward integration.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
	`t` (`realtype`) value of the independent variable at which y is desired (input).
	`y` (`N_Vector`) forward solution $y(t)$.
	`yp` (`N_Vector`) forward solution derivative $\dot{y}(t)$.
Return value	The return value `flag` (of type `int`) is one of:
	`IDA_SUCCESS` `IDAGetAdjY` was successful.
	`IDA_MEM_NULL` `ida_mem` was NULL.
	`IDA_GETY_BADT` The value of `t` was outside the current checkpoint interval.
Notes	The user must allocate space for `y` and `yp`.
F2003 Name	`FIDAGetAdjY`

IDAGetAdjCheckPointsInfo

Call	`flag = IDAGetAdjCheckPointsInfo(ida_mem, IDAadjCheckPointRec *ckpnt);`
Description	The function `IDAGetAdjCheckPointsInfo` loads an array of `ncheck+1` records of type `IDAadjCheckPointRec`. The user must allocate space for the array `ckpnt`.
Arguments	`ida_mem` (`void *`) pointer to the IDAS memory block created by `IDACreate`.
	`ckpnt` (`IDAadjCheckPointRec *`) array of `ncheck+1` checkpoint records, each of type `IDAadjCheckPointRec`.
Return value	The return value is `IDA_SUCCESS` if successful, or `IDA_MEM_NULL` if `ida_mem` is NULL, or `IDA_NO_ADJ` if ASA was not initialized.
Notes	The members of each record `ckpnt[i]` are:

- `ckpnt[i].my_addr` (`void *`) address of current checkpoint in `ida_mem->ida_adj_mem`
- `ckpnt[i].next_addr` (`void *`) address of next checkpoint
- `ckpnt[i].t0` (`realtype`) start of checkpoint interval

- ckpnt[i].t1 (`realtype`) end of checkpoint interval
- ckpnt[i].nstep (`long int`) step counter at ckeckpoint t0
- ckpnt[i].order (`int`) method order at checkpoint t0
- ckpnt[i].step (`realtype`) step size at checkpoint t0

F2003 Name `FIDAGetAdjCheckPointsInfo`

6.2.11.2 Initial condition calculation optional output function

`IDAGetConsistentICB`

Call   flag = IDAGetConsistentICB(ida_mem, which, yB0_mod, ypB0_mod);

Description   The function `IDAGetConsistentICB` returns the corrected initial conditions for backward problem calculated by `IDACalcICB`.

Arguments   ida_mem   (`void *`) pointer to the IDAS memory block.
             which   is the identifier of the backward problem.
             yB0_mod   (`N_Vector`) consistent initial vector.
             ypB0_mod (`N_Vector`) consistent initial derivative vector.

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

             IDA_SUCCESS   The optional output value has been successfully set.
             IDA_MEM_NULL   The ida_mem pointer is NULL.
             IDA_NO_ADJ   IDAAdjInit has not been previously called.
             IDA_ILL_INPUT Parameter which did not refer a valid backward problem identifier.

Notes   If the consistent solution vector or consistent derivative vector is not desired, pass NULL for the corresponding argument.

             The user must allocate space for yB0_mod and ypB0_mod (if not NULL).

F2003 Name `FIDAGetConsistentICB`

6.2.12 Backward integration of quadrature equations

Not only the backward problem but also the backward quadrature equations may or may not depend on the forward sensitivities. Accordingly, one of the `IDAQuadInitB` or `IDAQuadInitBS` should be used to allocate internal memory and to initialize backward quadratures. For any other operation (extraction, optional input/output, reinitialization, deallocation), the same function is called regardless of whether or not the quadratures are sensitivity-dependent.

6.2.12.1 Backward quadrature initialization functions

The function `IDAQuadInitB` initializes and allocates memory for the backward integration of quadrature equations that do not depende on forward sensititvities. It has the following form:

`IDAQuadInitB`

Call   flag = IDAQuadInitB(ida_mem, which, rhsQB, yQB0);

Description   The function `IDAQuadInitB` provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.

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

rhsQB	(IDAQuadRhsFnB) is the C function which computes fQB, the residual of the backward quadrature equations. This function has the form rhsQB(t, y, yp, yB, ypB, rhsvalBQ, user_dataB) (see §6.3.3).
yQB0	(N_Vector) is the value of the quadrature variables at tB0.

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

IDA_SUCCESS	The call to IDAQuadInitB was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_ADJ	The function IDAAdjInit has not been previously called.
IDA_MEM_FAIL	A memory allocation request has failed.
IDA_ILL_INPUT	The parameter which is an invalid identifier.

F2003 Name   FIDAQuadInitB

The function IDAQuadInitBS initializes and allocates memory for the backward integration of quadrature equations that depend on the forward sensitivities.

<u>IDAQuadInitBS</u>

Call	flag = IDAQuadInitBS(ida_mem, which, rhsQBS, yQBS0);
Description	The function IDAQuadInitBS provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.
Arguments	ida_mem (void *) pointer to the IDAS memory block.
	which (int) the identifier of the backward problem.
	rhsQBS (IDAQuadRhsFnBS) is the C function which computes $fQBS$, the residual of the backward quadrature equations. This function has the form rhsQBS(t, y, yp, yS, ypS, yB, ypB, rhsvalBQS, user_dataB) (see §6.3.4).
	yQBS0 (N_Vector) is the value of the sensitivity-dependent quadrature variables at tB0.

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

IDA_SUCCESS	The call to IDAQuadInitBS was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_ADJ	The function IDAAdjInit has not been previously called.
IDA_MEM_FAIL	A memory allocation request has failed.
IDA_ILL_INPUT	The parameter which is an invalid identifier.

F2003 Name   FIDAQuadInitBS

The integration of quadrature equations during the backward phase can be re-initialized by calling the following function. Before calling IDAQuadReInitB for a new backward problem, call any desired solution extraction functions IDAGet** associated with the previous backward problem.

<u>IDAQuadReInitB</u>

Call	flag = IDAQuadReInitB(ida_mem, which, yQB0);
Description	The function IDAQuadReInitB re-initializes the backward quadrature integration.
Arguments	ida_mem (void *) pointer to the IDAS memory block.
	which (int) the identifier of the backward problem.
	yQB0 (N_Vector) is the value of the quadrature variables at tB0.

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

IDA_SUCCESS	The call to IDAQuadReInitB was successful.
IDA_MEM_NULL	ida_mem was NULL.
IDA_NO_ADJ	The function IDAAdjInit has not been previously called.

	IDA_MEM_FAIL	A memory allocation request has failed.
	IDA_NO_QUAD	Quadrature integration was not activated through a previous call to IDAQuadInitB.
	IDA_ILL_INPUT	The parameter `which` is an invalid identifier.

Notes   `IDAQuadReInitB` can be used after a call to either `IDAQuadInitB` or `IDAQuadInitBS`.

F2003 Name   `FIDAQuadReInitB`

6.2.12.2   Backward quadrature extraction function

To extract the values of the quadrature variables at the last return time of `IDASolveB`, IDAS provides a wrapper for the function `IDAGetQuad` (see §4.7.3). The call to this function has the form

---
IDAGetQuadB

Call   `flag = IDAGetQuadB(ida_mem, which, &tret, yQB);`

Description   The function `IDAGetQuadB` returns the quadrature solution vector after a successful return from `IDASolveB`.

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

            `tret`   (`realtype`) the time reached by the solver (output).

            `yQB`   (`N_Vector`) the computed quadrature vector.

Return value   The return value `flag` of `IDAGetQuadB` is one of:

	IDA_SUCCESS	`IDAGetQuadB` was successful.
	IDA_MEM_NULL	`ida_mem` is NULL.
	IDA_NO_ADJ	The function `IDAAdjInit` has not been previously called.
	IDA_NO_QUAD	Quadrature integration was not initialized.
	IDA_BAD_DKY	`yQB` was NULL.
	IDA_ILL_INPUT	The parameter `which` is an invalid identifier.

Notes   The user must allocate space for `yQB`.

          To obtain the quadratures associated with a given backward problem at some other time within the last integration step, first obtain a pointer to the proper IDAS memory structure by calling `IDAGetAdjIDABmem` and then use it to call `IDAGetQuadDky`.

F2003 Name   `FIDAGetQuadB`

6.2.12.3   Optional input/output functions for backward quadrature integration

Optional values controlling the backward integration of quadrature equations can be changed from their default values through calls to one of the following functions which are wrappers for the corresponding optional input functions defined in §4.7.4. The user must specify the identifier `which` of the backward problem for which the optional values are specified.

```
flag = IDASetQuadErrConB(ida_mem, which, errconQ);
flag = IDAQuadSStolerancesB(ida_mem, which, reltolQ, abstolQ);
flag = IDAQuadSVtolerancesB(ida_mem, which, reltolQ, abstolQ);
```

Their return value `flag` (of type `int`) can have any of the return values of its counterparts, but it can also be `IDA_NO_ADJ` if the function `IDAAdjInit` has not been previously called or `IDA_ILL_INPUT` if the parameter `which` was an invalid identifier.

     Access to optional outputs related to backward quadrature integration can be obtained by calling the corresponding `IDAGetQuad*` functions (see §4.7.5). A pointer `ida_memB` to the IDAS memory block for the backward problem, required as the first argument of these functions, can be obtained through a call to the functions `IDAGetAdjIDABmem` (see §6.2.11).

6.3   User-supplied functions for adjoint sensitivity analysis

In addition to the required DAE residual function and any optional functions for the forward problem, when using the adjoint sensitivity module in IDAS, the user must supply one function defining the backward problem DAE and, optionally, functions to supply Jacobian-related information and one or two functions that define the preconditioner (if applicable for the choice of SUNLINSOL object) for the backward problem. Type definitions for all these user-supplied functions are given below.

6.3.1   DAE residual for the backward problem

The user must provide a `resB` function of type `IDAResFnB` defined as follows:

`IDAResFnB`

Definition	`typedef int (*IDAResFnB)(realtype t, N_Vector y, N_Vector yp,`
	                         `N_Vector yB, N_Vector ypB,`
	                         `N_Vector resvalB, void *user_dataB);`

Purpose	This function evaluates the residual of the backward problem DAE system. This could be (2.20) or (2.25).
Arguments	t is the current value of the independent variable.
	y is the current value of the forward solution vector.
	yp is the current value of the forward solution derivative vector.
	yB is the current value of the backward dependent variable vector.
	ypB is the current value of the backward dependent derivative vector.
	resvalB is the output vector containing the residual for the backward DAE problem.
	user_dataB is a pointer to user data, same as passed to `IDASetUserDataB`.
Return value	An `IDAResFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if an unrecoverabl failure occurred (in which case the integration stops and `IDASolveB` returns `IDA_RESFUNC_FAIL`).
Notes	Allocation of memory for `resvalB` is handled within IDAS.

The y, yp, yB, ypB, and `resvalB` arguments are all of type `N_Vector`, but yB, ypB, and `resvalB` typically have different internal representations from y and yp. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their `N_Vector` arguments (see §9.3 and §9.4).

The `user_dataB` pointer is passed to the user's `resB` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `resB` function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the residual function which will halt the integration and `IDASolveB` will return `IDA_RESFUNC_FAIL`.

6.3.2   DAE residual for the backward problem depending on the forward sensitivities

The user must provide a `resBS` function of type `IDAResFnBS` defined as follows:

IDAResFnBS

Definition	`typedef int (*IDAResFnBS)(realtype t, N_Vector y, N_Vector yp,`
	`                          N_Vector *yS, N_Vector *ypS,`
	`                          N_Vector yB, N_Vector ypB,`
	`                          N_Vector resvalB, void *user_dataB);`

Purpose   This function evaluates the residual of the backward problem DAE system. This could be (2.20) or (2.25).

Arguments
t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yp	is the current value of the forward solution derivative vector.
yS	a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
ypS	a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.
yB	is the current value of the backward dependent variable vector.
ypB	is the current value of the backward dependent derivative vector.
resvalB	is the output vector containing the residual for the backward DAE problem.
user_dataB	is a pointer to user data, same as passed to `IDASetUserDataB`.

Return value   An `IDAResFnBS` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if an unrecoverable error occurred (in which case the integration stops and `IDASolveB` returns `IDA_RESFUNC_FAIL`).

Notes   Allocation of memory for `resvalB` is handled within IDAS.

The y, yp, yB, ypB, and `resvalB` arguments are all of type `N_Vector`, but yB, ypB, and `resvalB` typically have different internal representations from y and yp. Likewise for each `yS[i]` and `ypS[i]`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with respect to their `N_Vector` arguments (see §9.3 and §9.4).

The `user_dataB` pointer is passed to the user's `resBS` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `resBS` function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the residual function which will halt the integration and `IDASolveB` will return `IDA_RESFUNC_FAIL`.

6.3.3 Quadrature right-hand side for the backward problem

The user must provide an `fQB` function of type `IDAQuadRhsFnB` defined by

---

IDAQuadRhsFnB

Definition	`typedef int (*IDAQuadRhsFnB)(realtype t, N_Vector y, N_Vector yp,`
	`                             N_Vector yB, N_Vector ypB,`
	`                             N_Vector rhsvalBQ, void *user_dataB);`

Purpose   This function computes the quadrature equation right-hand side for the backward problem.

Arguments
t	is the current value of the independent variable.
y	is the current value of the forward solution vector.

yp   is the current value of the forward solution derivative vector.

yB   is the current value of the backward dependent variable vector.

ypB   is the current value of the backward dependent derivative vector.

rhsvalBQ   is the output vector containing the residual for the backward quadrature
                equations.

user_dataB is a pointer to user data, same as passed to `IDASetUserDataB`.

Return value   An `IDAQuadRhsFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDASolveB` returns `IDA_QRHSFUNC_FAIL`).

Notes   Allocation of memory for `rhsvalBQ` is handled within IDAS.

                The y, yp, yB, ypB, and `rhsvalBQ` arguments are all of type `N_Vector`, but they typically all have different internal representations. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with repsect to their `N_Vector` arguments (see §9.3 and §9.4).

                The `user_dataB` pointer is passed to the user's `fQB` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

                Before calling the user's `fQB` function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and `IDASolveB` will return `IDA_QRHSFUNC_FAIL`.

6.3.4 Sensitivity-dependent quadrature right-hand side for the backward problem

The user must provide an `fQBS` function of type `IDAQuadRhsFnBS` defined by

---

`IDAQuadRhsFnBS`

Definition   ```
                typedef int (*IDAQuadRhsFnBS)(realtype t, N_Vector y, N_Vector yp,
                                              N_Vector *yS, N_Vector *ypS,
                                              N_Vector yB, N_Vector ypB,
                                              N_Vector rhsvalBQS, void *user_dataB);
                ```

Purpose   This function computes the quadrature equation residual for the backward problem.

Arguments   t   is the current value of the independent variable.

                y   is the current value of the forward solution vector.

                yp   is the current value of the forward solution derivative vector.

                yS   a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.

                ypS   a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.

                yB   is the current value of the backward dependent variable vector.

                ypB   is the current value of the backward dependent derivative vector.

                rhsvalBQS is the output vector containing the residual for the backward quadrature equations.

                user_dataB is a pointer to user data, same as passed to `IDASetUserDataB`.

Return value An `IDAQuadRhsFnBS` should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `IDASolveB` returns `IDA_QRHSFUNC_FAIL`).

Notes   Allocation of memory for `rhsvalBQS` is handled within IDAS.

The `y`, `yp`, `yB`, `ypB`, and `rhsvalBQS` arguments are all of type `N_Vector`, but they typically do not all have the same internal representations. Likewise for each `yS[i]` and `ypS[i]`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with IDAS do not perform any consistency checks with repsect to their `N_Vector` arguments (see §9.3 and §9.4).

The `user_dataB` pointer is passed to the user's `fQBS` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `fQBS` function, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and `IDASolveB` will return `IDA_QRHSFUNC_FAIL`.

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

If a matrix-based linear solver module is is used for the backward problem (i.e., `IDASetLinearSolverB` is called with non-`NULL` SUNMATRIX argument in the step described in §6.1), the user may provide a function of type `IDALsJacFnB` or `IDALsJacFnBS` (see §6.2.10), defined as follows:

`IDALsJacFnB`

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

Purpose   This function computes the Jacobian of the backward problem (or an approximation to it).

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

              `cjB`   is the scalar in the system Jacobian, proportional to the inverse of the step size (α in Eq. (2.6)).

              `yy`   is the current value of the forward solution vector.

              `yp`   is the current value of the forward solution derivative vector.

              `yB`   is the current value of the backward dependent variable vector.

              `ypB`   is the current value of the backward dependent derivative vector.

              `resvalB`   is the current value of the residual for the backward problem.

              `JacB`   is the output approximate Jacobian matrix.

              `user_dataB` is a pointer to user data — the parameter passed to `IDASetUserDataB`.

              `tmp1B`

              `tmp2B`

              `tmp3B`   are pointers to memory allocated for variables of type `N_Vector` which can be used by the `IDALsJacFnB` function as temporary storage or work space.

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

Notes   A user-supplied Jacobian function must load the matrix `JacB` with an approximation to the Jacobian matrix at the point (`tt`,`yy`,`yB`), where `yy` is the solution of the original IVP at time `tt`, and `yB` is the solution of the backward problem at the same time. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 10 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 `JacB`.

                Before calling the user's `IDALsJacFnB`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL` and IDALS sets `last_flag` to `IDALS_JACFUNC_UNRECVR`).

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

`IDALsJacFnBS`

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

Purpose         This function computes the Jacobian of the backward problem (or an approximation to it), in the case where the backward problem depends on the forward sensitivities.

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

                `cjB`       is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ).

                `yy`        is the current value of the forward solution vector.

                `yp`        is the current value of the forward solution derivative vector.

                `yS`        a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.

                `ypS`       a pointer to an array of `Ns` vectors containing the derivatives of the forward solution sensitivities.

                `yB`        is the current value of the backward dependent variable vector.

                `ypB`       is the current value of the backward dependent derivative vector.

                `resvalB`   is the current value of the residual for the backward problem.

                `JacB`      is the output approximate Jacobian matrix.

                `user_dataB` is a pointer to user data — the parameter passed to `IDASetUserDataB`.

                `tmp1B`

                `tmp2B`

| | |
|---|---|
| | **tmp3B** are pointers to memory allocated for variables of type **N_Vector** which can be used by **IDALsJacFnBS** as temporary storage or work space. |
| Return value | An **IDALsJacFnBS** should return 0 if successful, a positive value if a recoverable error occurred (in which case IDAS will attempt to correct, while IDALS sets **last_flag** to **IDALS_JACFUNC_RECVR**), or a negative value if it failed unrecoverably (in which case the integration is halted, **IDASolveB** returns **IDA_LSETUP_FAIL** and IDALS sets **last_flag** to **IDALS_JACFUNC_UNRECVR**). |
| Notes | A user-supplied dense Jacobian function must load the matrix **JacB** with an approximation to the Jacobian matrix at the point (**tt,yy,yS,yB**), where **yy** is the solution of the original IVP at time **tt**, **yS** is the array of forward sensitivities at time **tt**, and **yB** is the solution of the backward problem at the same time. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 10 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 **JacB**. |
| | Before calling the user's **IDALsJacFnBS**, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the Jacobian function which will halt the integration (**IDASolveB** returns **IDA_LSETUP_FAIL** and IDALS sets **last_flag** to **IDALS_JACFUNC_UNRECVR**). |
| | The previous function type **IDADlsJacFnBS** is identical to **IDALsJacFnBS**, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon. |

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

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

---

| IDALsJacTimesVecFnB |
|---|

| | |
|---|---|
| Definition | `typedef int (*IDALsJacTimesVecFnB)(realtype t,` <br>         `N_Vector yy, N_Vector yp,` <br>         `N_Vector yB, N_Vector ypB,` <br>         `N_Vector resvalB,` <br>         `N_Vector vB, N_Vector JvB,` <br>         `realtype cjB, void *user_dataB,` <br>         `N_Vector tmp1B, N_Vector tmp2B);` |
| Purpose | This function computes the action of the backward problem Jacobian **JB** on a given vector **vB**. |
| Arguments | **t** is the current value of the independent variable. |
| | **yy** is the current value of the forward solution vector. |
| | **yp** is the current value of the forward solution derivative vector. |
| | **yB** is the current value of the backward dependent variable vector. |
| | **ypB** is the current value of the backward dependent derivative vector. |

resvalB      is the current value of the residual for the backward problem.

vB           is the vector by which the Jacobian must be multiplied.

JvB          is the computed output vector, JB*vB.

cjB          is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ).

user_dataB   is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.

tmp1B

tmp2B        are pointers to memory allocated for variables of type N_Vector which can be used by IDALsJacTimesVecFnB as temporary storage or work space.

Return value The return value of a function of type IDALsJtimesVecFnB should be 0 if successful or nonzero if an error was encountered, in which case the integration is halted.

Notes        A user-supplied Jacobian-vector product function must load the vector JvB with the product of the Jacobian of the backward problem at the point (t, y, yB) and the vector vB. Here, y is the solution of the original IVP at time t and yB is the solution of the backward problem at the same time. The rest of the arguments are equivalent to those passed to a function of type IDALsJacTimesVecFn (see §4.6.6). If the backward problem is the adjoint of $\dot{y} = f(t, y)$, then this function is to compute $-(\partial f/\partial y)^T v_B$.

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

---

| IDALsJacTimesVecFnBS |

Definition   typedef int (*IDALsJacTimesVecFnBS)(realtype t,
                                                 N_Vector yy, N_Vector yp,
                                                 N_Vector *yyS, N_Vector *ypS,
                                                 N_Vector yB, N_Vector ypB,
                                                 N_Vector resvalB,
                                                 N_Vector vB, N_Vector JvB,
                                                 realtype cjB, void *user_dataB,
                                                 N_Vector tmp1B, N_Vector tmp2B);

Purpose      This function computes the action of the backward problem Jacobian JB on a given vector vB, in the case where the backward problem depends on the forward sensitivities.

Arguments    t            is the current value of the independent variable.

             yy           is the current value of the forward solution vector.

             yp           is the current value of the forward solution derivative vector.

             yyS          a pointer to an array of Ns vectors containing the sensitivities of the forward solution.

             ypS          a pointer to an array of Ns vectors containing the derivatives of the forward sensitivities.

             yB           is the current value of the backward dependent variable vector.

             ypB          is the current value of the backward dependent derivative vector.

             resvalB      is the current value of the residual for the backward problem.

             vB           is the vector by which the Jacobian must be multiplied.

             JvB          is the computed output vector, JB*vB.

             cjB          is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ).

             user_dataB   is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.

| | | |
|---|---|---|
| | tmp1B | |
| | tmp2B | are pointers to memory allocated for variables of type N_Vector which can be used by IDALsJacTimesVecFnBS as temporary storage or work space. |

Return value  The return value of a function of type IDALsJtimesVecFnBS should be 0 if successful or nonzero if an error was encountered, in which case the integration is halted.

Notes  A user-supplied Jacobian-vector product function must load the vector JvB with the product of the Jacobian of the backward problem at the point (t, y, yB) and the vector vB. Here, y is the solution of the original IVP at time t and yB is the solution of the backward problem at the same time. The rest of the arguments are equivalent to those passed to a function of type IDALsJacTimesVecFn (see §4.6.6).

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

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

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

| IDALsJacTimesSetupFnB |
|---|

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

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

Arguments  
tt        is the current value of the independent variable.

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

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

yB        is the current value of the backward dependent variable vector.

ypB       is the current value of the backward dependent derivative vector.

resvalB   is the current value of the residual for the backward problem.

cjB       is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ).

user_dataB is a pointer to user data — the same as the user_dataB parameter passed to IDASetUserDataB.

Return value  The value returned by the Jacobian-vector setup function should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

If the user's IDALsJacTimesVecFnB function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize,

the error weights, etc. To obtain these, the user will need to add a pointer to `ida_mem` to `user_dataB` and then use the `IDAGet*` functions described in §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

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

---

| `IDALsJacTimesSetupFnBS` |
|---|

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

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

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

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

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

                   `yyS`         a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.

                   `ypS`         a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities.

                   `yB`          is the current value of the backward dependent variable vector.

                   `ypB`         is the current value of the backward dependent derivative vector.

                   `resvalB`    is the current value of the residual for the backward problem.

                   `cjB`         is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ).

                   `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `IDASetUserDataB`.

Return value    The value returned by the Jacobian-vector setup function should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

If the user's `IDALsJacTimesVecFnB` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current stepsize, the error weights, etc. To obtain these, the user will need to add a pointer to `ida_mem` to `user_dataB` and then use the `IDAGet*` functions described in §4.5.10.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

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

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

If preconditioning is used during integration of the backward problem, then the user must provide a function to solve the linear system $Pz = r$, where $P$ is a left preconditioner matrix. This function must have one of the following two forms:

---

IDALsPrecSolveFnB

| | |
|---|---|
| Definition | `typedef int (*IDALsPrecSolveFnB)(realtype t,`<br>`                                 N_Vector yy, N_Vector yp,`<br>`                                 N_Vector yB, N_Vector ypB,`<br>`                                 N_Vector resvalB,`<br>`                                 N_Vector rvecB, N_Vector zvecB,`<br>`                                 realtype cjB, realtype deltaB,`<br>`                                 void *user_dataB);` |

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

Arguments
| | |
|---|---|
| `t` | is the current value of the independent variable. |
| `yy` | is the current value of the forward solution vector. |
| `yp` | is the current value of the forward solution derivative vector. |
| `yB` | is the current value of the backward dependent variable vector. |
| `ypB` | is the current value of the backward dependent derivative vector. |
| `resvalB` | is the current value of the residual for the backward problem. |
| `rvecB` | is the right-hand side vector $r$ of the linear system to be solved. |
| `zvecB` | is the computed output vector. |
| `cjB` | is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ). |
| `deltaB` | is an input tolerance to be used if an iterative method is employed in the solution. |
| `user_dataB` | is a pointer to user data — the same as the `user_dataB` parameter passed to the function `IDASetUserDataB`. |

Return value   The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

---

IDALsPrecSolveFnBS

| | |
|---|---|
| Definition | `typedef int (*IDALsPrecSolveFnBS)(realtype t,`<br>`                                  N_Vector yy, N_Vector yp,`<br>`                                  N_Vector *yyS, N_Vector *ypS,`<br>`                                  N_Vector yB, N_Vector ypB,`<br>`                                  N_Vector resvalB,`<br>`                                  N_Vector rvecB, N_Vector zvecB,`<br>`                                  realtype cjB, realtype deltaB,`<br>`                                  void *user_dataB);` |

Purpose    This function solves the preconditioning system $Pz = r$ for the backward problem, for the case in which the backward problem depends on the forward sensitivities.

Arguments
| | |
|---|---|
| `t` | is the current value of the independent variable. |
| `yy` | is the current value of the forward solution vector. |

|            |                                                                                           |
| ---------- | ----------------------------------------------------------------------------------------- |
| yp         | is the current value of the forward solution derivative vector.                           |
| yyS        | a pointer to an array of Ns vectors containing the sensitivities of the forward solution. |
| ypS        | a pointer to an array of Ns vectors containing the derivatives of the forward sensitivities. |
| yB         | is the current value of the backward dependent variable vector.                           |
| ypB        | is the current value of the backward dependent derivative vector.                         |
| resvalB    | is the current value of the residual for the backward problem.                            |
| rvecB      | is the right-hand side vector $r$ of the linear system to be solved.                      |
| zvecB      | is the computed output vector.                                                            |
| cjB        | is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ). |
| deltaB     | is an input tolerance to be used if an iterative method is employed in the solution.      |
| user_dataB | is a pointer to user data — the same as the user_dataB parameter passed to the function IDASetUserDataB. |

Return value   The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

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

If the user's preconditioner requires that any Jacobian-related data be preprocessed or evaluated, then this needs to be done in a user-supplied function of one of the following two types:

IDALsPrecSetupFnB

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

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

Arguments    The arguments of an IDALsPrecSetupFnB are as follows:

|            |                                                                             |
| ---------- | --------------------------------------------------------------------------- |
| t          | is the current value of the independent variable.                           |
| yy         | is the current value of the forward solution vector.                        |
| yp         | is the current value of the forward solution vector.                        |
| yB         | is the current value of the backward dependent variable vector.             |
| ypB        | is the current value of the backward dependent derivative vector.           |
| resvalB    | is the current value of the residual for the backward problem.              |
| cjB        | is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ). |
| user_dataB | is a pointer to user data — the same as the user_dataB parameter passed to the function IDASetUserDataB. |

Return value   The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

---

`IDALsPrecSetupFnBS`

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

Purpose   This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments   The arguments of an `IDALsPrecSetupFnBS` are as follows:

| | |
|---|---|
| `t` | is the current value of the independent variable. |
| `yy` | is the current value of the forward solution vector. |
| `yp` | is the current value of the forward solution vector. |
| `yyS` | a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution. |
| `ypS` | a pointer to an array of `Ns` vectors containing the derivatives of the forward sensitivities. |
| `yB` | is the current value of the backward dependent variable vector. |
| `ypB` | is the current value of the backward dependent derivative vector. |
| `resvalB` | is the current value of the residual for the backward problem. |
| `cjB` | is the scalar in the system Jacobian, proportional to the inverse of the step size ($\alpha$ in Eq. (2.6) ). |
| `user_dataB` | is a pointer to user data — the same as the `user_dataB` parameter passed to the function `IDASetUserDataB`. |

Return value   The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

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

## 6.4   Using the band-block-diagonal preconditioner for backward problems

As on the forward integration phase, the efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. The band-block-diagonal preconditioner module IDABBDPRE, provides interface functions through which it can be used on the backward integration phase.

The adjoint module in IDAS offers an interface to the band-block-diagonal preconditioner module IDABBDPRE described in section §4.8. This generates a preconditioner that is a block-diagonal matrix with each block being a band matrix and can be used with one of the Krylov linear solvers and with the MPI-parallel vector module NVECTOR_PARALLEL.

In order to use the IDABBDPRE module in the solution of the backward problem, the user must define one or two additional functions, described at the end of this section.

### 6.4.1  Usage of IDABBDPRE for the backward problem

The IDABBDPRE module is initialized by calling the following function, *after* an iterative linear solver for the backward problem has been attached to IDAS by calling `IDASetLinearSolverB` (see §6.2.6).

---

| IDABBDPrecInitB |
|---|

Call
`flag = IDABBDPrecInitB(ida_mem, which, NlocalB, mudqB, mldqB, mukeepB, mlkeepB, dqrelyB, GresB, GcommB);`

Description   The function `IDABBDPrecInitB` initializes and allocates memory for the IDABBDPRE preconditioner for the backward problem.

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

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

 `NlocalB` (`sunindextype`) local vector dimension for the backward problem.

 `mudqB`   (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.

 `mldqB`   (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.

 `mukeepB` (`sunindextype`) upper half-bandwidth of the retained banded approximate Jacobian block.

 `mlkeepB` (`sunindextype`) lower half-bandwidth of the retained banded approximate Jacobian block.

 `dqrelyB` (`realtype`) the relative increment in components of `yB` used in the difference quotient approximations. The default is `dqrelyB=`$\sqrt{\text{unit roundoff}}$, which can be specified by passing `dqrely=` 0.0.

 `GresB`   (`IDABBDLocalFnB`) the C function which computes $G_B(t, y, \dot{y}, y_B, \dot{y}_B)$, the function approximating the residual of the backward problem.

 `GcommB`  (`IDABBDCommFnB`) the optional C function which performs all interprocess communication required for the computation of $G_B$.

Return value  If successful, `IDABBDPrecInitB` creates, allocates, and stores (internally in the IDAS solver block) a pointer to the newly created IDABBDPRE memory block. The return value `flag` (of type `int`) is one of:

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

 `IDALS_MEM_FAIL`  A memory allocation request has failed.

 `IDALS_MEM_NULL`  The `ida_mem` argument was `NULL`.

 `IDALS_LMEM_NULL` No linear solver has been attached.

 `IDALS_ILL_INPUT` An invalid parameter has been passed.

F2003 Name  `FIDABBDPrecInitB`

To reinitialize the IDABBDPRE preconditioner module for the backward problem, possibly with a change in `mudqB`, `mldqB`, or `dqrelyB`, call the following function:

---

IDABBDPrecReInitB

Call      `flag = IDABBDPrecReInitB(ida_mem, which, mudqB, mldqB, dqrelyB);`

Description   The function `IDABBDPrecReInitB` reinitializes the IDABBDPRE preconditioner for the backward problem.

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

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

   `mudqB`   (`sunindextype`) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.

   `mldqB`   (`sunindextype`) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.

   `dqrelyB` (`realtype`) the relative increment in components of yB used in the difference quotient approximations.

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

   IDALS_SUCCESS    The call to `IDABBDPrecReInitB` was successful.

   IDALS_MEM_FAIL   A memory allocation request has failed.

   IDALS_MEM_NULL   The `ida_mem` argument was `NULL`.

   IDALS_PMEM_NULL  The `IDABBDPrecInitB` has not been previously called.

   IDALS_LMEM_NULL  No linear solver has been attached.

   IDALS_ILL_INPUT  An invalid parameter has been passed.

F2003 Name   FIDABBDPrecReInitB

For more details on IDABBDPRE see §4.8.

## 6.4.2   User-supplied functions for IDABBDPRE

To use the IDABBDPRE module, the user must supply one or two functions which the module calls to construct the preconditioner: a required function `GresB` (of type `IDABBDLocalFnB`) which approximates the residual of the backward problem and which is computed locally, and an optional function `GcommB` (of type `IDABBDCommFnB`) which performs all interprocess communication necessary to evaluate this approximate residual (see §4.8). The prototypes for these two functions are described below.

---

IDABBDLocalFnB

Definition   ```
typedef int (*IDABBDLocalFnB)(sunindextype NlocalB, realtype t,
                              N_Vector y, N_Vector yp,
                              N_Vector yB, N_Vector ypB,
                              N_Vector gB, void *user_dataB);
```

Purpose   This `GresB` function loads the vector `gB`, an approximation to the residual of the backward problem, as a function of `t`, `y`, `yp`, and `yB` and `ypB`.

Arguments   `NlocalB`   is the local vector length for the backward problem.

   `t`   is the value of the independent variable.

   `y`   is the current value of the forward solution vector.

   `yp`   is the current value of the forward solution derivative vector.

   `yB`   is the current value of the backward dependent variable vector.

   `ypB`   is the current value of the backward dependent derivative vector.

   `gB`   is the output vector, $G_B(t, y, \dot{y}, y_B, \dot{y}_B)$.

   `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `IDASetUserDataB`.

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

Notes This routine must assume that all interprocess communication of data needed to calculate `gB` has already been done, and this data is accessible within `user_dataB`.

Before calling the user's `IDABBDLocalFnB`, IDAS needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, IDAS triggers an unrecoverable failure in the preconditioner setup function which will halt the integration (`IDASolveB` returns `IDA_LSETUP_FAIL`).

| `IDABBDCommFnB` |

Definition `typedef int (*IDABBDCommFnB)(sunindextype NlocalB, realtype t,`
`N_Vector y, N_Vector yp,`
`N_Vector yB, N_Vector ypB,`
`void *user_dataB);`

Purpose This `GcommB` function performs all interprocess communications necessary for the execution of the `GresB` function above, using the input vectors y, yp, yB and ypB.

Arguments `NlocalB`   is the local vector length.

`t`   is the value of the independent variable.

`y`   is the current value of the forward solution vector.

`yp`   is the current value of the forward solution derivative vector.

`yB`   is the current value of the backward dependent variable vector.

`ypB`   is the current value of the backward dependent derivative vector.

`user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `IDASetUserDataB`.

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

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

Each call to the `GcommB` function is preceded by a call to the function that evaluates the residual of the backward problem with the same t, y, yp, yB and ypB arguments. If there is no additional communication needed, then pass `GcommB = NULL` to `IDABBDPrecInitB`.

Chapter 7

Using IDAS for Fortran Applications

A Fortran 2003 module (`fidas_mod`) is provided to support the use of IDAS, for the solution of DAE systems and performing forward sensitivity analysis or adjoint sensitivity analysis in a mixed Fortran/C setting. While IDAS is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in Fortran.

7.1   IDAS Fortran 2003 Interface Module

The `fidas_mod` Fortran module defines interfaces to most IDAS 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 IDAS function `IDACreate` is interfaced as `FIDACreate`. Thus, the steps to use IDAS 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 Chapters 4, 5, and 6 . The Fortran 2003 IDAS interface module can be accessed by the `use` statement, i.e. `use fidas_mod`, and linking to the library `libsundials_fidas_mod.`*lib* in addition to `libsundials_idas.`*lib*.

The Fortran 2003 interface modules were generated with SWIG Fortran, a fork of SWIG [42]. Users who are interested in the SWIG code used in the generation process should contact the SUNDIALS *development team.*

7.1.1   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 7.1). 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 7.1.3. A discussion on the topic of equivalent data types in C and Fortran 2003 is presented in section 7.1.2.

Further information on the Fortran 2003 interfaces specific to modules is given in the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL alongside the C documentation (chapters 9, 10, 11, and

12 respectively). For details on where the Fortran 2003 module (`.mod`) files and libraries are installed see Appendix A.

Table 7.1: 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`

7.1.2   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 7.2 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.

Table 7.2: 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)

7.1.3   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 7.1.2 discusses equivalencies of data types in the two languages.

7.1.3.1   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.

7.1.3.2   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)
```

7.1.3.3   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.

7.1.3.4   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 7.1.2), 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)
```

7.1.3.5   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 9.1.6.

7.1.3.6   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.

$\boxed{\texttt{FSUNDIALSFileClose}}$

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

7.1.4   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.

Chapter 8

IDAS Features for GPU Accelerated Computing

This chapter is concerned with using GPU-acceleration and IDAS for the integration of DAEs, forward sensitivity analysis, and adjoint sensitivity analysis.

8.1 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 §9, §10, §11, and §12) 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 §9.15) 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 8.1 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 §13.1 to support applications which implement their own memory management or memory pooling.

Table 8.1: 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 (§9.9)	✓			✓	✓
NVECTOR_RAJA (§9.11)	✓			✓	✓
NVECTOR_OPENMPDEV (§9.13)	✓	✓	✓	✓	
SUNMATRIX_CUSPARSE (§10.7)	✓			✓	✓
SUNLINSOL_CUSOLVERSP_BATCHQR (§11.12)	✓			✓	✓
SUNLINSOL_SPGMR (§11.14)	†	†	†	†	†
SUNLINSOL_SPFGMR (§11.15)	†	†	†	†	†
SUNLINSOL_SPTFQMR (§11.17)	†	†	†	†	†
SUNLINSOL_SPBCGS (§11.16)	†	†	†	†	†
SUNLINSOL_PCG (§11.18)	†	†	†	†	†
SUNNONLINSOL_NEWTON (§12.3)	†	†	†	†	†
SUNNONLINSOL_FIXEDPOINT (§??)	†	†	†	†	†

8.2   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 8.1 for a list of GPU-enabled native SUNDIALS modules.

Chapter 9

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.

9.1 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.

9.1.1 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 9.1.
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`

$\boxed{\texttt{N\_VGetDeviceArrayPointer}}$

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`

$\boxed{\texttt{N\_VSetArrayPointer}}$

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`

$\boxed{\texttt{N\_VGetCommunicator}}$

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`

$\boxed{\texttt{N\_VGetLength}}$

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 (success-
ful 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 num_i by $denom_i$. A zero element in `denom` will be skipped. If no such quotients are found, then the large value `BIG_REAL` (defined in the header file `sundials_types.h`) is returned.

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`

9.1.2   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)
```

9.1.3   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.

9.1.4 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 9.16). 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:

$$m = \max_{0 \leq i < n_{local}} |x_i|,$$

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:

$$m = \min_{0 \leq i < n_{local}} x_i,$$

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 num_i by $denom_i$, for all MPI task-local components of the vectors. A zero element in `denom` will be skipped. If no such quotients are found, then the large value `BIG_REAL` (defined in the header file `sundials_types.h`) is returned.

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`

9.1.5   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`

9.1.6   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 exist-
                 ing 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 9.1: 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`

9.1.7   NVECTOR identifiers

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 9.1.

9.1.8   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 9.1.1 defines a complete list of all standard vector operations defined by the generic NVECTOR module. Sections 9.1.2, 9.1.3 and 9.1.4 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
```

9.1.9   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.

9.1.9.1   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 9.1.1-9.1.4 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., $m = \min_i \mathrm{real}(x_i)$.

- 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.

9.2   NVECTOR functions used by IDAS

In Table 9.2 below, we list the vector functions used in the NVECTOR module used by the IDAS package. The table also shows, for each function, which of the code modules uses the function. The IDAS column shows function usage within the main integrator module, while the remaining columns show function

usage within the IDAS linear solvers interface, the IDABBDPRE preconditioner module, and the IDAA module.

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

Special cases (numbers match markings in table):

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

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

3. The optional function N_VDotProdMulti is only used when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR. The remaining operations from Tables 9.1.2 and 9.1.3 not listed above are unused and a user-supplied NVECTOR module for IDAS could omit these operations.

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

Of the functions listed in Table 9.1.1, N_DotProd, N_VWL2Norm, N_VL1Norm, N_VInvTest, and N_VGetCommunicator are *not* used by IDAS. Therefore a user-supplied NVECTOR module for IDAS could omit these functions (although some may be needed by SUNNONLINSOL or SUNLINSOL modules).

9.3 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.

9.3.1 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] )
  ```

9.3.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3 and 9.1.4. 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 9.1.1 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 For-
tran 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.

9.3.3   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.

9.4   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.

9.4.1 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] )
  ```

9.4.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4. 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 inter-
              face 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 For-
              tran 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.

9.4.3   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.

9.5   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 NVEC-TOR_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.

9.5.1   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] )
  ```

9.5.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4. 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 9.1.1 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.

9.5.3   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.

9.6   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.

9.6.1   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] )
  ```

9.6.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4. 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 9.1.1 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.

9.6.3   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 func-
tions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interop-
erating 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.

9.7   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.

9.7.1   NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 [40] and the `ark_diurnal_kry_ph.c` example program for ARKODE [50].

The names of parhyp methods are obtained from those in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 op-
              eration 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.

9.8   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.

9.8.1   NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 [38].

     The names of vector operations are obtained from those in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 implementa-
              tions.

N_VMake_Petsc

Prototype   N_Vector N_VMake_Petsc(Vec *pvec)

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

N_VGetVector_Petsc

Prototype   Vec *N_VGetVector_Petsc(N_Vector v)

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

N_VCloneVectorArray_Petsc

Prototype   N_Vector *N_VCloneVectorArray_Petsc(int count, N_Vector w)

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

N_VCloneVectorArrayEmpty_Petsc

Prototype   N_Vector *N_VCloneVectorArrayEmpty_Petsc(int count, N_Vector w)

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

N_VDestroyVectorArray_Petsc

Prototype   void N_VDestroyVectorArray_Petsc(N_Vector *vs, int count)

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

N_VPrint_Petsc

Prototype   void N_VPrint_Petsc(N_Vector v)

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

N_VPrintFile_Petsc

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

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

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

N_VEnableFusedOps_Petsc

Prototype   int N_VEnableFusedOps_Petsc(N_Vector v, booleantype tf)

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

N_VEnableLinearCombination_Petsc

Prototype   int N_VEnableLinearCombination_Petsc(N_Vector v, booleantype tf)

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

N_VEnableScaleAddMulti_Petsc

Prototype   int N_VEnableScaleAddMulti_Petsc(N_Vector v, booleantype tf)

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

N_VEnableDotProdMulti_Petsc

Prototype   int N_VEnableDotProdMulti_Petsc(N_Vector v, booleantype tf)

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

N_VEnableLinearSumVectorArray_Petsc

Prototype   int N_VEnableLinearSumVectorArray_Petsc(N_Vector v, booleantype tf)

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

N_VEnableScaleVectorArray_Petsc

Prototype   int N_VEnableScaleVectorArray_Petsc(N_Vector v, booleantype tf)

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

N_VEnableConstVectorArray_Petsc

Prototype   int N_VEnableConstVectorArray_Petsc(N_Vector v, booleantype tf)

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

N_VEnableWrmsNormVectorArray_Petsc

Prototype   int N_VEnableWrmsNormVectorArray_Petsc(N_Vector v, booleantype tf)

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

N_VEnableWrmsNormMaskVectorArray_Petsc

Prototype   int N_VEnableWrmsNormMaskVectorArray_Petsc(N_Vector v, booleantype tf)

Description This function enables (SUNTRUE) or disables (SUNFALSE) the masked WRMS norm 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.

9.9 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.

9.9.1   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 9.1.1, 9.1.2, 9.1.3 and 9.1.4, 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 [40].

The names of vector operations are obtained from those in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 (num-
              ber of thread blocks) is a multiple of the CUDA warp size (32). See section 9.9.2 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_VSetKernelExecPolicy_Cuda
              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 op-
eration 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.

9.9.2 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.

9.10   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.

9.10.1 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 9.1.1, 9.1.2, 9.1.3 and 9.1.4, except for `N_VSetArrayPointer`. The names of vector operations are obtained from those in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 9.10.2 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.

9.10.2 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.

9.11   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.

9.11.1   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 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 [40].

The names of vector operations are obtained from those in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 op-
              erations 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.

9.12 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.

9.12.1 NVECTOR_SYCL functions

The NVECTOR_SYCL module implementations of all vector operations listed in the sections in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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.

$\boxed{\texttt{N\_VSetHostArrayPointer\_Sycl}}$

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.

$\boxed{\texttt{N\_VSetDeviceArrayPointer\_Sycl}}$

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.

$\boxed{\texttt{N\_VCopyToDevice\_Sycl}}$

Prototype   `realtype *N_VCopyToDevice_Sycl(N_Vector v)`

Description   This function copies host vector data to the device.

$\boxed{\texttt{N\_VCopyFromDevice\_Sycl}}$

Prototype   `realtype *N_VCopyFromDevice_Sycl(N_Vector v)`

Description   This function copies vector data from the device to the host.

$\boxed{\texttt{N\_VIsManagedMemory\_Sycl}}$

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.

$\boxed{\texttt{N\_VSetKernelExecPolicy\_Sycl}}$

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 9.12.2 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.

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

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.

9.12.2   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.

9.13   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.

9.13.1   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 )
```

9.13.2   NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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.

9.14   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.

9.14.1   NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in Tables 9.1.1, 9.1.4, and 9.1.4, 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 [38].

The names of vector operations are obtained from those in Tables 9.1.1, 9.1.4, and 9.1.4 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 recommended 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.

9.15   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.

9.15.1   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.

9.15.2   NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 7.1.3.5, and the functions are documented in Chapter 9.1.6.

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 For-
             tran 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 op-
             eration for vector arrays in the ManyVector. The return value is 0 for success and -1 if
             the input vector or its ops structure are NULL.

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.

9.16 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 9.1.4.

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.

9.16.1 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.

9.16.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, 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 9.1.1, 9.1.2, 9.1.3, and 9.1.4 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 7.1.3.5, and the functions are documented in Chapter 9.1.6.

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 us-
                ing 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 For-
                tran 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 op-
                erations 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 For-
                tran 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.

9.17 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.

9.17.1 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 9.16.1.

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.

9.17.2 NVECTOR_MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in Tables 9.1.1, 9.1.2, 9.1.3, and 9.1.4, from the NVECTOR_MPIMANYVECTOR (see section 9.16.2) 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:

$\boxed{\texttt{N\_VMake\_MPIPlusX}}$

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.

$\boxed{\texttt{N\_VGetLocalVector\_MPIPlusX}}$

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.

$\boxed{\texttt{N\_VGetArrayPointer\_MPIPlusX}}$

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.

$\boxed{\texttt{N\_VSetArrayPointer\_MPIPlusX}}$

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.

9.18   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.

Table 9.2: List of vector functions usage by IDAS code modules

	IDAS	IDALS	IDABBDPRE	IDAA
N_VGetVectorID				
N_VGetLength		4		
N_VClone	✓	✓	✓	✓
N_VCloneEmpty		1		
N_VDestroy	✓	✓	✓	✓
N_VCloneVectorArray	✓			✓
N_VDestroyVectorArray	✓			✓
N_VSpace	✓	2		
N_VGetArrayPointer		1	✓	
N_VSetArrayPointer		1		
N_VLinearSum	✓	✓		✓
N_VConst	✓	✓		✓
N_VProd	✓			
N_VDiv	✓			
N_VScale	✓	✓	✓	✓
N_VAbs	✓			
N_VInv	✓			
N_VAddConst	✓			
N_VMaxNorm	✓			
N_VWrmsNorm	✓	✓		
N_VMin	✓			
N_VMinQuotient	✓			
N_VConstrMask	✓			
N_VWrmsNormMask	✓			
N_VCompare	✓			
N_VLinearCombination	✓			
N_VScaleAddMulti	✓			
N_VDotProdMulti		3		
N_VLinearSumVectorArray	✓			
N_VScaleVectorArray	✓			
N_VConstVectorArray	✓			
N_VWrmsNormVectorArray	✓			
N_VWrmsNormMaskVectorArray	✓			
N_VScaleAddMultiVectorArray	✓			
N_VLinearCombinationVectorArray	✓			

Chapter 10

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.

10.1 The SUNMatrix API

The SUNMATRIX API can be grouped into two sets of functions: the core matrix operations, and utility functions. Section 10.1.1 lists the core operations, while Section 10.1.2 lists the utility functions.

10.1.1 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 10.2.
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`

10.1.2   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

10.1.3   SUNMatrix return codes

The functions provided to SUNMATRIX modules within the SUNDIALS-provided SUNMATRIX implementa-
tions utilize a common set of return codes, shown in Table 10.1. 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 10.1: Description of the SUNMatrix return codes

Name	Value	Description
SUNMAT_SUCCESS	0	successful call or converged solve
		continued on next page

Table 10.2: 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

10.1.4 SUNMatrix identifiers

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 10.2. It is recommended that a user-supplied SUNMATRIX implementation use the SUNMATRIX_CUSTOM identifier.

10.1.5 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 11. More specifically, in Table 10.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 10.3: 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	✓	✓	✓	✓	✓	✓	✓	✓	✓

10.1.6 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 10.1.1 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
```

10.1.7 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 10.1.2.

10.2 SUNMatrix functions used by IDAS

In Table 10.4, we list the matrix functions in the SUNMATRIX module used within the IDAS package. The table also shows, for each function, which of the code modules uses the function. The main IDAS integrator does not call any SUNMATRIX functions directly, so the table columns are specific to the IDALS interface and the IDABBDPRE preconditioner module. We further note that the IDALS interface only utilizes these routines when supplied with a *matrix-based* linear solver, i.e., the SUNMATRIX object passed to IDASetLinearSolver was not NULL.

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

Table 10.4: List of matrix functions usage by IDAS code modules

	IDALS	IDABBDPRE
SUNMatGetID	✓	
SUNMatDestroy		✓
SUNMatZero	✓	✓
SUNMatSpace		†

The matrix functions listed in Section 10.1.1 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 10.1.1 that are *not* used by IDAS

are: SUNMatCopy, SUNMatClone, SUNMatScaleAdd, SUNMatScaleAddI and SUNMatMatvec. Therefore a user-supplied SUNMATRIX module for IDAS could omit these functions.

10.3 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 $0 \leq$ i $<$ M and $0 \leq$ 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 $0 \leq$ i $<$ M and $0 \leq$ j $<$ N) may be accessed via cols[j][i].

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

10.3.1 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 $M \times N$ dense matrix A (with $0 \leq j < N$). The type of the expression `SM_COLUMN_D(A,j)` is `realtype *`. The pointer returned by the call `SM_COLUMN_D(A,j)` can be treated as an array which is indexed from 0 to $M - 1$.

  The assignments `SM_ELEMENT_D(A,i,j) = a_ij` and `a_ij = SM_ELEMENT_D(A,i,j)` reference the (i,j)-th element of the $M \times N$ dense matrix A (with $0 \leq i < M$ and $0 \leq j < N$).

  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] )
```

10.3.2 SUNMatrix_Dense functions

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Section 10.1.1. Their names are obtained from those in Section 10.1.1 by appending the suffix _Dense (e.g. SUNMatCopy_Dense). All the standard matrix operations listed in Section 10.1.1 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.

10.3.3   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.

10.4   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 10.1. A more complete description of the parts of this *content* field is given below:

M   - number of rows

N   - number of columns (`N` = `M`)

mu   - upper half-bandwidth, $0 \leq$ `mu` $<$ `N`

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

s_mu   - storage upper bandwidth, `mu` $\leq$ `s_mu` $<$ `N`. The LU decomposition routines in the associated SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(`N`-1,`mu+ml`) because of partial pivoting. The `s_mu` field holds the upper half-bandwidth allocated for A.

ldim   - leading dimension (`ldim` $\geq$ `s_mu+ml+1`)

data   - pointer to a contiguous block of `realtype` variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. `data` is a pointer to `ldata` contiguous locations which hold the elements within the band of A.

ldata   - length of the data array ($=$ `ldim`$\cdot N$)

cols   - array of pointers. `cols[j]` is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from `s_mu−mu` (to access the uppermost element within the band in the j-th column) to `s_mu+ml` (to access the lowest element within the band in the j-th column). Indices from 0 to `s_mu−mu−1` give access to extra storage elements required by the LU decomposition function. Finally, `cols[j][i-j+s_mu]` is the (i, j)-th element with j−`mu` $\leq i \leq j$+`ml`.

The header file to include when using this module is `sunmatrix/sunmatrix_band.h`. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixband` module library.

10.4.1   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 )
  ```
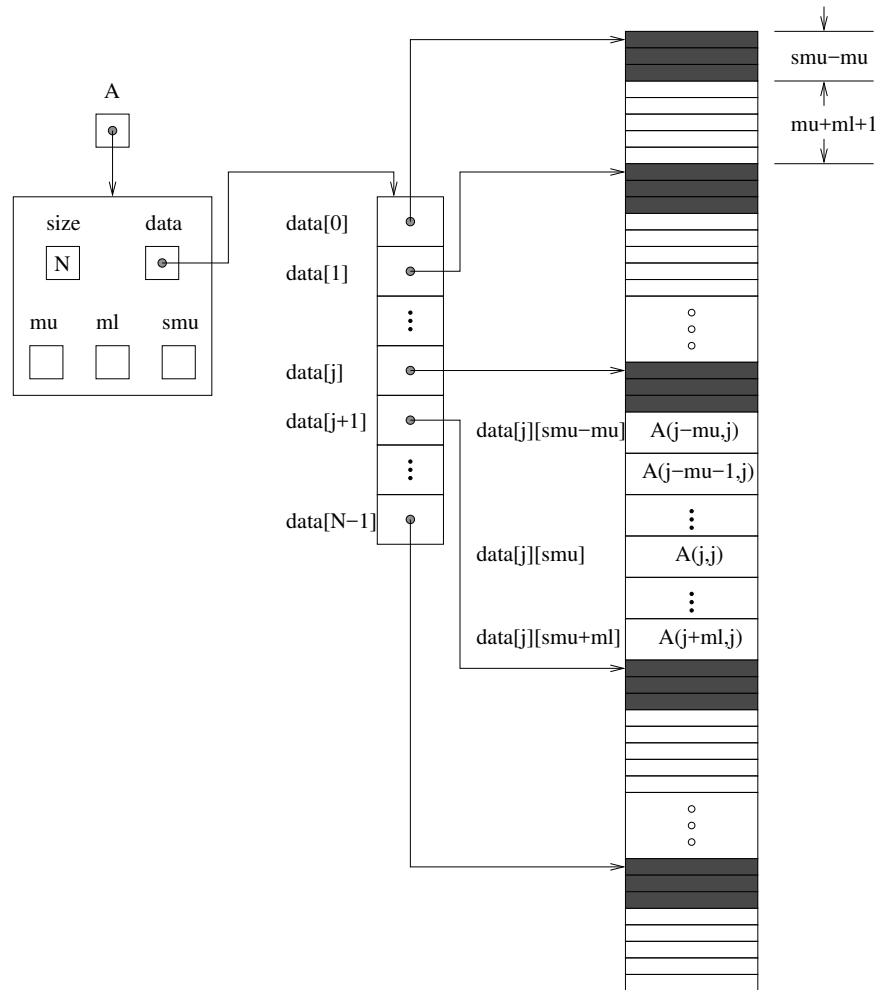
Figure 10.1: Diagram of the storage for the SUNMATRIX_BAND module. Here A is an N × N band matrix with upper and lower half-bandwidths mu and ml, respectively. The rows and columns of A are numbered from 0 to N − 1 and the (i, j)-th element of A is denoted A(i,j). The greyed out areas of the underlying component storage are used by the associated SUNLINSOL_BAND linear solver.

```
#define SM_SUBAND_B(A)       ( SM_CONTENT_B(A)->s_mu )

#define SM_LDIM_B(A)         ( SM_CONTENT_B(A)->ldim )

#define SM_LDATA_B(A)        ( SM_CONTENT_B(A)->ldata )
```

- SM_DATA_B and SM_COLS_B

  These macros give access to the `data` and `cols` pointers for the matrix entries.

  The assignment `A_data = SM_DATA_B(A)` sets `A_data` to be a pointer to the first component of the data array for the banded `SUNMatrix A`. The assignment `SM_DATA_B(A) = A_data` sets the data array of `A` to be `A_data` by storing the pointer `A_data`.

  Similarly, the assignment `A_cols = SM_COLS_B(A)` sets `A_cols` to be a pointer to the array of column pointers for the banded `SUNMatrix A`. The assignment `SM_COLS_B(A) = A_cols` sets the column pointer array of `A` to be `A_cols` by storing the pointer `A_cols`.

  Implementation:

```
#define SM_DATA_B(A)         ( SM_CONTENT_B(A)->data )

#define SM_COLS_B(A)         ( SM_CONTENT_B(A)->cols )
```

- SM_COLUMN_B, SM_COLUMN_ELEMENT_B, and SM_ELEMENT_B

  These macros give access to the individual columns and entries of the data array of a banded `SUNMatrix`.

  The assignments `SM_ELEMENT_B(A,i,j) = a_ij` and `a_ij = SM_ELEMENT_B(A,i,j)` reference the (i,j)-th element of the $N \times N$ band matrix `A`, where $0 \le i, j \le N - 1$. The location (i,j) should further satisfy $j-mu \le i \le j+ml$.

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

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

  Implementation:

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

#define SM_COLUMN_ELEMENT_B(col_j,i,j) (col_j[(i)-(j)])

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

10.4.2   SUNMatrix_Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Section 10.1.1. Their names are obtained from those in Section 10.1.1 by appending the suffix _Band (e.g. SUNMatCopy_Band). All the standard matrix operations listed in Section 10.1.1 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 inter-
              face module.

Notes

- When looping over the components of a banded SUNMatrix A, the most efficient approaches are
  to:
  - First obtain the component array via A_data = SM_DATA_B(A) or
    A_data = SUNBandMatrix_Data(A) and then access A_data[i] within the loop.
  - First obtain the array of column pointers via A_cols = SM_COLS_B(A) or
    A_cols = SUNBandMatrix_Cols(A), and then access A_cols[j][i] within the loop.
  - Within a loop over the columns, access the column pointer via
    A_colj = SUNBandMatrix_Column(A,j) and then to access the entries within that column
    using SM_COLUMN_ELEMENT_B(A_colj,i,j).

All three of these are more efficient than using SM_ELEMENT_B(A,i,j) within a double loop.

- Within the SUNMatMatvec_Band routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

10.4.3   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.

10.5   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 10.2 (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 SUNMA-
TRIX_SPARSE module is accessible from all SUNDIALS solvers *without* linking to the
`libsundials_sunmatrixsparse` module library.

10.5.1   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 )
  ```

NULL   NULL

rowvals   colptrs   colvals   rowptrs   M   NP = N   N

A

indexvals   indexptrs   data   NNZ   sparsetype=CSC_MAT

0   →   A(*rowvals[0],0)

j   →   A(*rowvals[1],0)   column 0

⋮   ⋮   ⋮

k   →   A(*rowvals[j],1)

nz   ⋮

→   A(*rowvals[k],NP−1)

⋮   column NP−

A(*rowvals[nz−1],NP−1)

unused
storage
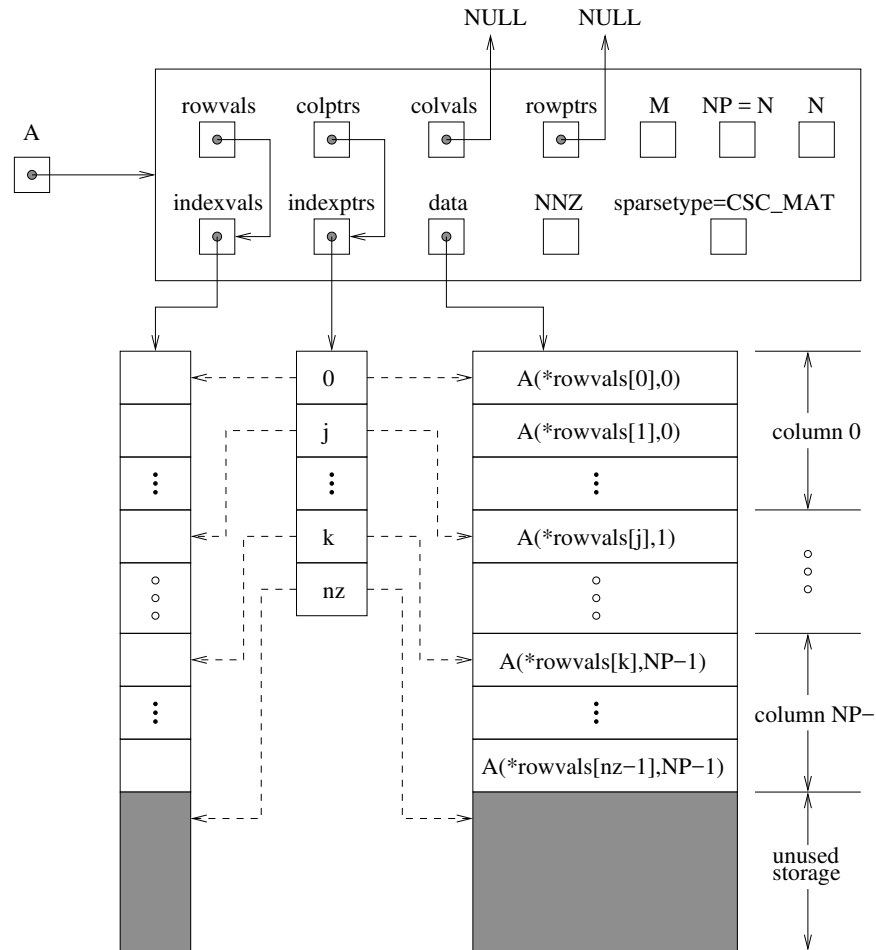
Figure 10.2: Diagram of the storage for a compressed-sparse-column matrix. Here A is an M × N sparse matrix with storage for up to NNZ nonzero entries (the allocated length of both data and indexvals). The entries in indexvals may assume values from 0 to M − 1, corresponding to the row index (zero-based) of each nonzero value. The entries in data contain the values of the nonzero entries, with the row i, column j entry of A (again, zero-based) denoted as A(i,j). The indexptrs array contains N + 1 entries; the first N denote the starting index of each column within the indexvals and data arrays, while the final entry points one past the final nonzero entry. Here, although NNZ values are allocated, only nz are actually filled in; the greyed-out portions of data and indexvals indicate extra allocated space.

- 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 )
    ```

10.5.2 SUNMatrix_Sparse functions

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Section 10.1.1. Their names are obtained from those in Section 10.1.1 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). All the standard matrix operations listed in Section 10.1.1 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 inter-
                 face 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.

10.5.3   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.

10.6   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, 31, 46, 47]. It is designed to be used with the SUNLINSOL_SUPERLUDIST linear solver discussed in Section 11.10. 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.

10.6.1 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 SUN-Matrix will wrap; must have `Stype = SLU_NR_loc, Dtype = SLU_D, Mtype = SLU_GE` to be compatible

`grid (gridinfo_t*)` the initialized SuperLU_DIST 2D process grid structure

Return value a `SUNMatrix` object if `Asuper` is compatible else `NULL`

Notes

SUNMatrix_SLUNRloc_Print

Call   `SUNMatrix_SLUNRloc_Print(A, fp);`

Description   The function `SUNMatrix_SLUNRloc_Print` prints the underlying `SuperMatrix` content.

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

Return value `void`

Notes

 SUNMatrix_SLUNRloc_SuperMatrix

Call   `Asuper = SUNMatrix_SLUNRloc_SuperMatrix(A);`

Description   The function `SUNMatrix_SLUNRloc_SuperMatrix` provides access to the underlying 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 10.1.1:

- `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.

10.7 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 11.12).

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. ⚠

10.7.1 SUNMatrix_cuSparse functions

The `SUNMATRIX_CUSPARSE` module defines GPU-enabled sparse implementations of all matrix operations listed in Section 10.1.1 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 9.9.2 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.

10.7.2   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.

10.8   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 [55]. 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.

10.8.1   SUNMATRIX_MAGMADENSE functions

The SUNMATRIX_MAGMADENSE module defines GPU-enabled implementations of all matrix operations listed in Section 10.1.1.

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 $M_{\mathrm{block}} \times$ 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 $N_{\mathrm{block}} \times$ 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

10.8.2 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 11

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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{11.1}$$

where

$$
\begin{aligned}
\tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\
\tilde{b} &= S_1 P_1^{-1} b, \\
\tilde{x} &= S_2 P_2 x,
\end{aligned}
\tag{11.2}
$$

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

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

We note that the corresponding adjustments to tol in this case are non-optimal, in that they cannot balance error between specific entries of the solution x, only the aggregate error in the overall solution vector.

We further note that not all of the SUNDIALS-provided iterative linear solvers support the full range of the above options (e.g., separate left/right preconditioning), and that some of the SUNDIALS packages only utilize a subset of these options. Further details on these exceptions are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS package.

For users interested in providing their own SUNLINSOL module, the following section presents the SUNLINSOL API and its implementation beginning with the definition of SUNLINSOL functions in sections 11.1.1 – 11.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 11.1.4. A table of linear solver return codes is given in section 11.1.5. The SUNLinearSolver type and the generic SUNLINSOL module are defined in section 11.1.6. The section 11.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 11.3 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 11.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

11.1   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`.

11.1.1   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 11.3.1 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 11.1.

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 11.1.
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 11.1.
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`

11.1.2 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 11.1.
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 (11.1)-(11.2). 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 11.1.
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 (11.1)-(11.2), 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 11.1.

F2003 Name FSUNLinSolSetScalingVectors

11.1.3　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 11.1.

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

F2003 Name `FSUNLinSolSpace`

11.1.4   Functions provided by SUNDIALS packages

To interface with the SUNLINSOL modules, the SUNDIALS packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic interfaces to the linear systems of equations that result in their solution. The types for functions provided to a SUNLINSOL module are defined in the header file `sundials/sundials_iterative.h`, and are described below.

`ATimesFn`

Definition   `typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);`

Purpose   These functions compute the action of a matrix on a vector, performing the operation $z = Av$. Memory for `z` should already be alloced prior to calling this function. The vector `v` should be left unchanged.

Arguments   `A_data` is a pointer to client data, the same as that supplied to `SUNLinSolSetATimes`.

             `v`   is the input vector to multiply.

             `z`   is the output vector computed.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

`PSetupFn`

Definition   `typedef int (*PSetupFn)(void *P_data)`

Purpose   These functions set up any requisite problem data in preparation for calls to the corresponding `PSolveFn`.

Arguments   `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

PSolveFn

Definition   typedef int (*PSolveFn)(void *P_data, N_Vector r, N_Vector z,
                                        realtype tol, int lr)

Purpose   These functions solve the preconditioner equation $Pz = r$ for the vector z. Memory for
              z should already be alloced prior to calling this function. The parameter P_data is a
              pointer to any information about P which the function needs in order to do its job (set
              up by the corresponding PSetupFn). The parameter lr is input, and indicates whether
              P is to be taken as the left preconditioner or the right preconditioner: lr $= 1$ for left
              and lr $= 2$ for right. If preconditioning is on one side only, lr can be ignored. If the
              preconditioner is iterative, then it should strive to solve the preconditioner equation so
              that

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

              where the weight vector for the WRMS norm may be accessed from the main package
              memory structure. The vector r should not be modified by the PSolveFn.

Arguments   P_data is a pointer to client data, the same pointer as that supplied to the routine
                      SUNLinSolSetPreconditioner.
              r   is the right-hand side vector for the preconditioner system.
              z   is the solution vector for the preconditioner system.
              tol   is the desired tolerance for an iterative preconditioner.
              lr   is flag indicating whether the routine should perform left (1) or right (2) pre-
                      conditioning.

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.

11.1.5 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
11.1. 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 11.1: 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)

11.1.6   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 11.1.1-11.1.3. 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
```

11.2   Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 11.2 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 11.2: 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	✓	✓	✓	✓	✓

11.3   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 11.4 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 struc-
               ture 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.

11.3.1   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 SUNMA-
TRIX and SUNLINSOL implementations. Sections 10.2 and 11.4 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 implemen-
tations, 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 10 and 11. *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 11.4.2 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, SUN-DIALS a user must implement a custom SUNLINSOL wrapper for the linear solver following the API described in Chapter 11. *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.

11.4 IDAS SUNLinearSolver interface

Table 11.3 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 11.3: 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	†	†	†

11.4.1 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

$$x = \frac{2}{1 + \alpha/\bar{\alpha}}\bar{x}. \tag{11.3}$$

The motivation for this selection of the scaling factor $c = 2/(1 + \alpha/\bar{\alpha})$ is discussed in detail in [11, 34].
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.

11.4.2 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 (11.1)-(11.2)):

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

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2 / \sqrt{n}$$

is computed and the scaled tolerance `delta`$= \text{tol}/W_{mean}$ is supplied to the SUNLINSOL object.

11.5   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.

11.5.1   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).

11.5.2   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 11.1.1 – 11.1.3:

- 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.

11.5.3   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.

11.5.4 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.

11.6 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.

11.6.1   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`.

11.6.2   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 :

- `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.

11.6.3   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.

11.6.4   SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a SUNLinearSolver as the following struc-
ture:

```
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.

11.7   The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LA-
PACK. The SUNLINSOL_LAPACKDENSE module is designed to be used with the corresponding SUNMA-
TRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVEC-
TOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

     To access the SUNLINSOL_LAPACKDENSE module, include the header file
sunlinsol/sunlinsol_lapackdense.h. The installed module library to link to is
libsundials_sunlinsollapackdense.*lib* where .*lib* is typically .so for shared libraries and .a for
static libraries.

     The SUNLINSOL_LAPACKDENSE module is a SUNLINSOL wrapper for the LAPACK dense matrix
factorization and solve routines, *GETRF and *GETRS, where * is either D or S, depending on whether
SUNDIALS was configured to have realtype set to double or single, respectively (see Section 4.2).
In order to use the SUNLINSOL_LAPACKDENSE module it is assumed that LAPACK has been installed
on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately
to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit
floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when
using extended precision for realtype. Similarly, since there do not exist 64-bit integer LAPACK
routines, the SUNLINSOL_LAPACKDENSE module also cannot be compiled when using 64-bit integers
for the sunindextype.

11.7.1   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).

11.7.2 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 11.1.1 – 11.1.3:

- `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`

11.7.3 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 ob-
ject.

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.

11.7.4   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.

11.8   The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LA-
PACK. The SUNLINSOL_LAPACKBAND module is designed to be used with the corresponding SUNMA-
TRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVEC-
TOR_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.

⚠

11.8.1 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.

⚠

11.8.2 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 11.1.1 – 11.1.3:

- 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

11.8.3   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.

11.8.4   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.

11.9   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, 24]. 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.

11.9.1   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.

11.9.2   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 11.1.1 – 11.1.3:

- 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 iden-
                     tial 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 SUNLIN-
                  SOL_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 com-
                 piled 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 SUNLIN-
                  SOL_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 com-
                 piled 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.

11.9.3 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.

11.9.4 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).

11.10 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.

11.10.1 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, 31, 46, 47]. 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 SUN-LINSOL_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.

11.10.2   SUNLinearSolver_SuperLUDIST functions

The SUNLINSOL_SUPERLUDIST module defines implementations of all "direct" linear solver operations listed in Sections 11.1.1-11.1.3:

- `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 struc-
                ture that contains the distributed L and U factors.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   LUstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSuperLUOptions

Call   superlu_dist_options_t *opts = SUNLinSol_SuperLUDIST_GetSuperLUOptions(LS);

Description   The function SUNLinSol_SuperLUDIST_GetSuperLUOptions returns the SuperLU_DIST
                structure that contains the options which control how the linear system is factorized
                and solved.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   superlu_dist_options_t*

Notes

SUNLinSol_SuperLUDIST_GetScalePermstruct

Call   ScalePermstruct_t *sp = SUNLinSol_SuperLUDIST_GetScalePermstruct(LS);

Description   The function SUNLinSol_SuperLUDIST_GetScalePermstruct returns the SuperLU_DIST
                structure that contains the vectors that describe the transformations done to the matrix,
                A.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   ScalePermstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSOLVEstruct

Call   SOLVEstruct_t *solve = SUNLinSol_SuperLUDIST_GetSOLVEstruct(LS);

Description   The function SUNLinSol_SuperLUDIST_GetSOLVEstruct returns the SuperLU_DIST struc-
                ture that contains information for communication during the solution phase.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   SOLVEstruct_t*

Notes

SUNLinSol_SuperLUDIST_GetSuperLUStat

Call   SuperLUStat_t *stat = SUNLinSol_SuperLUDIST_GetSuperLUStat(LS);

Description   The function SUNLinSol_SuperLUDIST_GetSuperLUStat returns the SuperLU_DIST struc-
                ture that stores information about runtime and flop count.

Arguments   LS (SUNLinearSolver) the SUNLINSOL_SUPERLUDIST object

Return value   SuperLUStat_t*

Notes

11.10.3   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

11.11   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, 45, 26]. 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.

11.11.1 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.

11.11.2 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 11.1.1 – 11.1.3:

- `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.

11.11.3 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.

11.11.4   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.

11.12   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.

11.12.1 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.

11.12.2 SUNLinearSolver_cuSolverSp_batchQR functions

The `SUNLinearSolver_cuSolverSp_batchQR` module defines implementations of all "direct" linear solver operations listed in Sections 11.1.1-11.1.3:

- `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 SUN-LINSOL 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 de-
            scription 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 descrip-
            tion 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

11.12.3   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            */
};
```

11.13   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 [55].

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.

11.13.1   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

$$
\begin{bmatrix}
\mathbf{A_0} & 0 & \cdots & 0 \\
0 & \mathbf{A_1} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \mathbf{A_{n-1}}
\end{bmatrix}
x_j = b_j.
$$

11.13.2   SUNLinearSolver_MagmaDense functions

The SUNLinearSolver_MagmaDense module defines implementations of all "direct" linear solver operations listed in Sections 11.1.1-11.1.3:

- 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.

11.13.3   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;
};
```

11.14   The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [52]) 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.

11.14.1   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.

11.14.2 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 11.1.1 – 11.1.3:

- 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

11.14.3 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 SUNLIN-SOL_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 SUN-LINSOL_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.

11.14.4   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 $v_1, \ldots, v_{\mathtt{maxl}+1}$, stored in V[0], ..., V[maxl]. Each v_i is a vector of type NVECTOR.,

Hes — the $(\mathtt{maxl} + 1) \times \mathtt{maxl}$ 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

11.15 The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [51]) 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.

11.15.1 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.

11.15.2 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 11.1.1 – 11.1.3:

- 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`

11.15.3   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 func-
tions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interop-
erating 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.

$\boxed{\text{FSUNSPFGMRINIT}}$

Call	FSUNSPFGMRINIT(code, pretype, maxl, ier)
Description	The function FSUNSPFGMRINIT can be called for Fortran programs to create a SUNLIN- SOL_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.

$\boxed{\text{FSUNMASSSPFGMRINIT}}$

Call	FSUNMASSSPFGMRINIT(pretype, maxl, ier)
Description	The function FSUNMASSSPFGMRINIT can be called for Fortran programs to create a SUN- LINSOL_SPFGMR object for mass matrix linear systems.
Arguments	pretype (int*) flag indicating desired preconditioning type
	maxl (int*) flag indicating Krylov subspace size
Return value	ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.
Notes	This routine must be called *after* the NVECTOR object has been initialized.
	Allowable values for pretype and maxl are the same as for the C function SUNLinSol_SPFGMR.

The SUNLinSol_SPFGMRSetPrecType, SUNLinSol_SPFGMRSetGSType and SUNLinSol_SPFGMRSetMaxRestarts routines also support Fortran interfaces for the system and mass matrix solvers.

$\boxed{\text{FSUNSPFGMRSETGSTYPE}}$

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.

$\boxed{\text{FSUNMASSSPFGMRSETGSTYPE}}$

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.

11.15.4   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] $= s_1, \ldots$ 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

11.16   The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [56]) 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.

11.16.1   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.

11.16.2 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 11.1.1 – 11.1.3:

- 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`

11.16.3   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.

11.16.4   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

11.17 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [30]) 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.

11.17.1 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.

11.17.2 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 identical 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 11.1.1 – 11.1.3:

- `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 identical 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

11.17.3   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 func-
tions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interop-
erating 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 in-
cludes 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 SUNLIN-
                SOL_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.

11.17.4 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

11.18   The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementaiton of the PCG (Preconditioned Conjugate Gradient [32]) 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.

11.18.1   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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{11.4}$$

where

$$
\begin{aligned}
\tilde{A} &= SP^{-1}AP^{-1}S, \\
\tilde{b} &= SP^{-1}b, \\
\tilde{x} &= S^{-1}Px.
\end{aligned}
\tag{11.5}
$$

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

$$\|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|SP^{-1}b - SP^{-1}Ax\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|P^{-1}b - P^{-1}Ax\|_S < \delta$$

where $\|v\|_S = \sqrt{v^T S^T S v}$, with an input tolerance δ.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_PCG to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s` scaling vector.

- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

11.18.2   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 11.1.1 – 11.1.3:

- `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

11.18.3   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 maxi-
               mum number of iterations to allow.

Arguments   code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for
                    KINSOL, and 4 for ARKODE).

               maxl (int*) the number of iterations to allow.

Return value   ier is a int return completion flag equal to 0 for a success return and -1 otherwise.
               See printed message for details in case of failure.

Notes   See SUNLinSol_PCGSetMaxl for complete further documentation of this routine.

| FSUNMASSPCGSETMAXL |

Call   FSUNMASSPCGSETMAXL(maxl, ier)

Description   The function FSUNMASSPCGSETMAXL can be called for Fortran programs to change the
               type of preconditioning for mass matrix linear systems.

Arguments   The arguments are identical to FSUNPCGSETMAXL above, except that code is not needed
               since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes   See `SUNLinSol_PCGSetMaxl` for complete further documentation of this routine.

11.18.4   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

11.19   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 12

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 12.2.

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 12.1 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 12.1.1 – 12.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 12.1.4. A table of nonlinear solver return codes is given in section 12.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 12.1.6. Section 12.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 12.1.8 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.

12.1 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`.

12.1.1 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 12.2 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 12.2 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

12.1.2 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 12.1.4 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 12.1.4 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 12.1.4 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 12.1.4 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 non-
               linear solver iterations. This is typically called by SUNDIALS integrators to define their
               default iteration limit, but may be adjusted by the user.

Arguments   NLS   (SUNNonlinearSolver) a SUNNONLINSOL object.

               maxiters   (int) the maximum number of nonlinear iterations.

Return value   The return value `retval` (of type `int`) should be zero for a successful call, and a negative
               value for a failure (e.g., `maxiters < 1`).

F2003 Name   FSUNNonlinSolSetMaxIters

12.1.3   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 non-
               linear solve. This function is *required* when using SUNDIALS integrator-provided conver-
               gence tests or when using a SUNLINSOL spils linear solver; otherwise it is *optional*.

Arguments   NLS   (SUNNonlinearSolver) a SUNNONLINSOL object

               iter   (int*) the nonlinear solver iteration in the current solve starting from zero.

Return value   The return value `retval` (of type `int`) should be zero for a successful call, and a negative
               value for a failure.

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`

12.1.4   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 12.2 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 12.2, 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).

$\boxed{\texttt{SUNNonlinSolLSolveFn}}$

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 implementa-
tions 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).

$\boxed{\texttt{SUNNonlinSolConvTestFn}}$

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 oc-
               curred or one of the following:

               SUN_NLS_SUCCESS   the iteration is converged.

               SUN_NLS_CONTINUE   the iteration has not converged, keep iterating.

               SUN_NLS_CONV_RECVR   the iteration appears to be diverging, try to recover.

Notes   The tolerance passed to this routine by SUNDIALS integrators is the tolerance in a
               weighted root-mean-squared norm with error weight vector `ewt`. SUNNONLINSOL mod-
               ules utilizing their own convergence criteria may ignore these functions.

12.1.5   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 12.1. Here, negative values correspond to non-recoverable failures, positive values to
recoverable failures, and zero to a successful call.

Table 12.1: 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

12.1.6   The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic SUN-
NONLINSOL module on which all other SUNNONLINSOL implementations are built. The
`SUNNonlinearSolver` type is a pointer to a structure containing an implementation-dependent *content*
field and an *ops* field. The type `SUNNonlinearSolver` is defined as follows:

```
typedef struct _generic_SUNNonlinearSolver *SUNNonlinearSolver;

struct _generic_SUNNonlinearSolver {
  void *content;
  struct _generic_SUNNonlinearSolver_Ops *ops;
};
```

where the `_generic_SUNNonlinearSolver_Ops` structure is a list of pointers to the various actual non-
linear solver operations provided by a specific implementation. The `_generic_SUNNonlinearSolver_Ops`
structure is defined as

```
struct _generic_SUNNonlinearSolver_Ops {
  SUNNonlinearSolver_Type (*gettype)(SUNNonlinearSolver);
  int                     (*initialize)(SUNNonlinearSolver);
  int                     (*setup)(SUNNonlinearSolver, N_Vector, void*);
  int                     (*solve)(SUNNonlinearSolver, N_Vector, N_Vector,
                                   N_Vector, realtype, booleantype, void*);
```

```
  int                   (*free)(SUNNonlinearSolver);
  int                   (*setsysfn)(SUNNonlinearSolver, SUNNonlinSolSysFn);
  int                   (*setlsetupfn)(SUNNonlinearSolver, SUNNonlinSolLSetupFn);
  int                   (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
  int                   (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn,
                                      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 12.1.1 – 12.1.3. 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
```

12.1.7 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 9.1.1 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

12.1.8 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 12.1.1 – 12.1.3. 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 struc-
              ture 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`

12.2 IDAS SUNNonlinearSolver interface

As discussed in Chapter 2 each integration step requires the (approximate) solution of the nonlinear
system

$$G(y_n) = F\left(t_n, y_n, h_n^{-1} \sum_{i=0}^{q} \alpha_{n,i} y_{n-i}\right) = 0. \tag{12.1}$$

Rather than solving this system for the new state y_n IDAS 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

$$G(y_{cor}) = F\left(t_n, y_{pred} + y_{cor}, \dot{y}_{pred} + \alpha y_{cor}\right) = 0. \tag{12.2}$$

where $\alpha = h_n^{-1}\alpha_{n,0}$. Similarly in the forward sensitivity analysis case the nonlinear system is also
reformulated in terms of the correction to the predicted sensitivities.

   The nonlinear system function provided by IDAS to the nonlinear solver module internally updates
the current value of the new state and its derivative based on the current corretion passed to the
function (as well as the sensitivities). These values are used when calling the DAE residual function
and when setting up linear solves (e.g., for updating the Jacobian or preconditioner).

   IDAS 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 Eq. 2.6).

Arguments   `ida_mem` (`void *`) pointer to the IDAS 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 IDAS 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 IDAS 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

| IDAGetCurrentYSens |

Call   **flag = IDAGetCurrentYSens(ida_mem, &yyS);**

Description The function **IDAGetCurrentYSens** returns the current sensitivity vector array.

Arguments   **ida_mem** (**void ***) pointer to the IDAS memory block.

yyS   (**N_Vector ****) pointer to the vector array that is set to the array of sensitivity vectors

Return value The return value **flag** (of type **int**) is one of

IDA_SUCCESS   The optional output value has been successfully set.

IDA_MEM_NULL The **ida_mem** pointer is NULL.

F2003 Name FIDAGetCurrentYSens

| IDAGetCurrentYpSens |

Call   **flag = IDAGetCurrentYpSens(ida_mem, &ypS);**

Description The function **IDAGetCurrentYpSens** returns the derivative the current sensitivity vector array.

Arguments   **ida_mem** (**void ***) pointer to the IDAS memory block.

ypS　　(N_Vector **) pointer to the vector array that is set to the array of sensitivity vector derivatives

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 FIDAGetCurrentYpSens

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 (12.2).

Arguments　ida_mem　(void *) pointer to the IDAS 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 (12.2)).

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 §12.1.4) 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 IDAS (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.,

$$yyn = y_{pred} + y_{cor},$$
$$ypn = \dot{y}_{pred} + \alpha \dot{y}_{cor},$$
$$res = F\left(t_n, y_n, \dot{y}_n\right),$$

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`

| `IDAGetNonlinearSystemDataSens` |

Call   `flag = IDAGetNonlinearSystemDataSens(ida_mem, &tcur, &yySpred, &ypSpred, &yySn, &ypSn, &cj, user_data);`

Description   The function `IDAGetNonlinearSystemDataSens` returns all internal sensitivity data required to construct the current nonlinear system (12.2).

Arguments   `ida_mem`   (`void *`) pointer to the IDAS memory block.

            `tcur`   (`realtype*`) current value of the independent variable t_n.

            `yySpred`   (`N_Vector**`) predicted value of $yS_{i,pred}$ at t_n for $i = 0 \ldots N_s - 1$.

            `ypSpred`   (`N_Vector**`) predicted value of $\dot{y}S_{i,pred}$ at t_n for $i = 0 \ldots N_s - 1$.

            `yySn`   (`N_Vector**`) the vectors $yS_{i,n}$. These vectors may be not current (see the note below).

            `ypSn`   (`N_Vector**`) the vectors $\dot{y}S_{i,n}$. These vectors may be not current (see the note below).

            `cj`   (`realtype*`) the scalar c_j which is proportional to the inverse of the step size (α in (12.2)).

            `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 §12.1.4) 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 `IDAGetNonlinearSystemDataSens` **inside** the nonlinear system function to access the requisite data for evaluting the nonlinear system function of their choosing. Additionlly, if the the vectors `yySn` and `ypSn` are provided as additional workspace and do not need to be filled in by the user's `SUNNonlinSolSysFn`.

            If this function is called as part of a custom linear solver (i.e., the default `SUNNonlinSolSysFn` is used) then the vectors `yySn` and `ypSn` are only current when `IDAGetNonlinearSystemDataSens` is called after an evaluation of the nonlinear system function.

F2003 Name `FIDAGetNonlinearSystemDataSens`

| `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 IDAS 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 $\dot{y}(t)$ based on the given correction vector from the nonlinear solver.

Arguments   `ida_mem` (`void *`) pointer to the IDAS 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`

`IDAComputeYSens`

Call   `flag = IDAComputeYSens(ida_mem, ycorS, yys);`

Description   The function computes the sensitivities based on the given correction vector from the nonlinear solver.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block

             `ycorS` (`N_Vector *`) the correction

             `yyS`   (`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   `FIDAComputeYSens`

`IDAComputeYpSens`

Call   `flag = IDAComputeYpSens(ida_mem, ycorS, ypS);`

Description   The function computes the sensitivity derivatives based on the given correction vector from the nonlinear solver.

Arguments   `ida_mem` (`void *`) pointer to the IDAS memory block

             `ycorS` (`N_Vector *`) the correction

             `ypS`   (`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   `FIDAComputeYpSens`

12.3   The SUNNonlinearSolver_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton's method. To access the SUNNON-LINSOL_NEWTON module, include the header file `sunnonlinsol/sunnonlinsol_newton.h`. We note that the SUNNONLINSOL_NEWTON module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolnewton` module library.

12.3.1 SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{12.3}$$

given an initial guess $y^{(0)}$, Newton's method computes a series of approximate solutions

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{12.4}$$

where m is the Newton iteration index, and the Newton update $\delta^{(m+1)}$ is the solution of the linear system

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)}) \,, \tag{12.5}$$

in which A is the Jacobian matrix

$$A \equiv \partial F / \partial y \,. \tag{12.6}$$

Depending on the linear solver used, the SUNNONLINSOL_NEWTON module will employ either a Modified Newton method, or an Inexact Newton method [12, 16, 25, 27, 43]. 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 `callLSetup` 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.

12.3.2 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 12.1.1 – 12.1.3
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 12.1.1 – 12.1.3 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 informa-
                tive (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`

12.3.3 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 sys-
                tems 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.

12.3.4   SUNNonlinearSolver_Newton content

The SUNNONLINSOL_NEWTON module defines the *content* field of a SUNNonlinearSolver as the fol-
lowing 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

12.4 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 9.8 which discusses the NVECTOR interface to the PETSc Vec API.

12.4.1 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.

12.4.2 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 12.1.1 – 12.1.3 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 12.1.1 – 12.1.3 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.

12.4.3   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 13

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.

13.1   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;
```

13.1.1   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).

13.1.2 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).

13.1.3 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.

13.1.4 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`.

13.2   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.

13.2.1   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).

13.3   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.

13.3.1   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).

13.4   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.

13.4.1 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
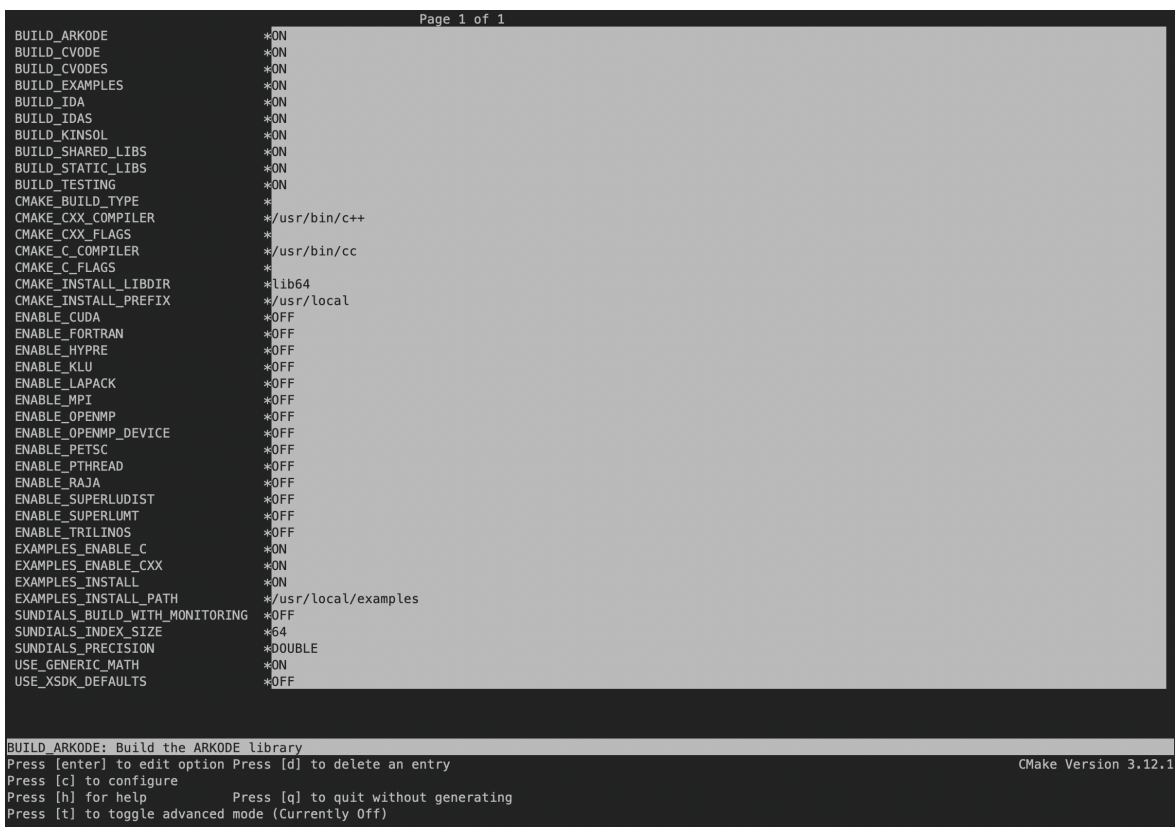
– For file and directories, the `<tab>` key can be used to complete

• 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
```

```
                                      Page 1 of 1
BUILD_ARKODE                    *ON
BUILD_CVODE                     *ON
BUILD_CVODES                    *ON
BUILD_EXAMPLES                  *ON
BUILD_IDA                       *ON
BUILD_IDAS                      *ON
BUILD_KINSOL                    *ON
BUILD_SHARED_LIBS               *ON
BUILD_STATIC_LIBS               *ON
BUILD_TESTING                   *ON
CMAKE_BUILD_TYPE                *
CMAKE_CXX_COMPILER              */usr/bin/c++
CMAKE_CXX_FLAGS                 *
CMAKE_C_COMPILER                */usr/bin/cc
CMAKE_C_FLAGS                   *
CMAKE_INSTALL_LIBDIR            *lib64
CMAKE_INSTALL_PREFIX            */usr/casc/sundials/instdir
ENABLE_CUDA                     *OFF
ENABLE_FORTRAN                  *OFF
ENABLE_HYPRE                    *OFF
ENABLE_KLU                      *OFF
ENABLE_LAPACK                   *OFF
ENABLE_MPI                      *OFF
ENABLE_OPENMP                   *OFF
ENABLE_OPENMP_DEVICE            *OFF
ENABLE_PETSC                    *OFF
ENABLE_PTHREAD                  *OFF
ENABLE_RAJA                     *OFF
ENABLE_SUPERLUDIST              *OFF
ENABLE_SUPERLUMT                *OFF
ENABLE_TRILINOS                 *OFF
EXAMPLES_ENABLE_C               *ON
EXAMPLES_ENABLE_CXX             *ON
EXAMPLES_INSTALL                *ON
EXAMPLES_INSTALL_PATH           */usr/casc/sundials/instdir/examples
SUNDIALS_BUILD_WITH_MONITORING  *OFF
SUNDIALS_INDEX_SIZE             *64
SUNDIALS_PRECISION              *DOUBLE
USE_GENERIC_MATH                *ON
USE_XSDK_DEFAULTS               *OFF




EXAMPLES_INSTALL_PATH: Output directory for installing example files
Press [enter] to edit option Press [d] to delete an entry                    CMake Version 3.12.1
Press [c] to configure
Press [h] for help          Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

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.*lib*
> 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 dep-
> recated. 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 dou-
> ble.
> 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
		continued on next page

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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*
continued on next page		

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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_impl.h
		cvode/cvode_direct.h cvode/cvode_ls.h
		cvode/cvode_spils.h cvode/cvode_bandpre.h
		cvode/cvode_bbdpre.h
	Module files	fcvode_mod.mod
CVODES	Libraries	libsundials_cvodes.*lib*
		libsundials_fcvodes_mod.*lib*
	Header files	cvodes/cvodes.h cvodes/cvodes_impl.h
		cvodes/cvodes_direct.h cvodes/cvodes_ls.h
		cvodes/cvodes_spils.h cvodes/cvodes_bandpre.h
		cvodes/cvodes_bbdpre.h
	Module files	fcvodes_mod.mod
ARKODE	Libraries	libsundials_arkode.*lib*
		libsundials_farkode.a
		libsundials_farkode_mod.*lib*
	Header files	arkode/arkode.h arkode/arkode_impl.h
		arkode/arkode_ls.h arkode/arkode_bandpre.h
		arkode/arkode_bbdpre.h
	Module files	farkode_mod.mod farkode_arkstep_mod.mod
		farkode_erkstep_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_impl.h
		ida/ida_direct.h ida/ida_ls.h
		ida/ida_spils.h ida/ida_bbdpre.h
	Module files	fida_mod.mod
continued on next page		

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IDAS	Libraries	libsundials_idas.*lib*	
		libsundials_fidas_mod.*lib*	
	Header files	idas/idas.h	idas/idas_impl.h
		idas/idas_direct.h	idas/idas_ls.h
		idas/idas_spils.h	idas/idas_bbdpre.h
	Module files	fidas_mod.mod	
KINSOL	Libraries	libsundials_kinsol.*lib*	
		libsundials_fkinsol.a	
		libsundials_fkinsol_mod.*lib*	
	Header files	kinsol/kinsol.h	kinsol/kinsol_impl.h
		kinsol/kinsol_direct.h	kinsol/kinsol_ls.h
		kinsol/kinsol_spils.h	kinsol/kinsol_bbdpre.h
	Module files	fkinsol_mod.mod	

Appendix B

IDAS Constants

Below we list all input and output constants used by the main solver and linear solver modules, together with their numerical values and a short description of their meaning.

B.1 IDAS input constants

IDAS **main solver module**		
IDA_NORMAL	1	Solver returns at specified output time.
IDA_ONE_STEP	2	Solver returns after each successful step.
IDA_SIMULTANEOUS	1	Simultaneous corrector forward sensitivity method.
IDA_STAGGERED	2	Staggered corrector forward sensitivity method.
IDA_CENTERED	1	Central difference quotient approximation (2nd order) of the sensitivity RHS.
IDA_FORWARD	2	Forward difference quotient approximation (1st order) of the sensitivity RHS.
IDA_YA_YDP_INIT	1	Compute y_a and $\dot{y}_d$, given y_d.
IDA_Y_INIT	2	Compute y, given $\dot{y}$.

IDAS **adjoint solver module**		
IDA_HERMITE	1	Use Hermite interpolation.
IDA_POLYNOMIAL	2	Use variable-degree polynomial interpolation.

Iterative linear solver module		
PREC_NONE	0	No preconditioning
PREC_LEFT	1	Preconditioning on the left.
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

B.2 IDAS output constants

IDAS **main solver module**		

IDA_SUCCESS	0	Successful function return.
IDA_TSTOP_RETURN	1	`IDASolve` succeeded by reaching the specified stopping point.
IDA_ROOT_RETURN	2	`IDASolve` succeeded and found one or more roots.
IDA_WARNING	99	`IDASolve` succeeded but an unusual situation occurred.
IDA_TOO_MUCH_WORK	-1	The solver took `mxstep` internal steps but could not reach tout.
IDA_TOO_MUCH_ACC	-2	The solver could not satisfy the accuracy demanded by the user for some internal step.
IDA_ERR_FAIL	-3	Error test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_CONV_FAIL	-4	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
IDA_LINIT_FAIL	-5	The linear solver's initialization function failed.
IDA_LSETUP_FAIL	-6	The linear solver's setup function failed in an unrecoverable manner.
IDA_LSOLVE_FAIL	-7	The linear solver's solve function failed in an unrecoverable manner.
IDA_RES_FAIL	-8	The user-provided residual function failed in an unrecoverable manner.
IDA_REP_RES_FAIL	-9	The user-provided residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_RTFUNC_FAIL	-10	The rootfinding function failed in an unrecoverable manner.
IDA_CONSTR_FAIL	-11	The inequality constraints were violated and the solver was unable to recover.
IDA_FIRST_RES_FAIL	-12	The user-provided residual function failed recoverably on the first call.
IDA_LINESEARCH_FAIL	-13	The line search failed.
IDA_NO_RECOVERY	-14	The residual function, linear solver setup function, or linear solver solve function had a recoverable failure, but `IDACalcIC` could not recover.
IDA_NLS_INIT_FAIL	-15	The nonlinear solver's init routine failed.
IDA_NLS_SETUP_FAIL	-16	The nonlinear solver's setup routine failed.
IDA_MEM_NULL	-20	The `ida_mem` argument was NULL.
IDA_MEM_FAIL	-21	A memory allocation failed.
IDA_ILL_INPUT	-22	One of the function inputs is illegal.
IDA_NO_MALLOC	-23	The IDAS memory was not allocated by a call to `IDAInit`.
IDA_BAD_EWT	-24	Zero value of some error weight component.
IDA_BAD_K	-25	The k-th derivative is not available.
IDA_BAD_T	-26	The time t is outside the last step taken.
IDA_BAD_DKY	-27	The vector argument where derivative should be stored is NULL.
IDA_NO_QUAD	-30	Quadratures were not initialized.
IDA_QRHS_FAIL	-31	The user-provided right-hand side function for quadratures failed in an unrecoverable manner.
IDA_FIRST_QRHS_ERR	-32	The user-provided right-hand side function for quadratures failed in an unrecoverable manner on the first call.

IDA_REP_QRHS_ERR	-33	The user-provided right-hand side repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_NO_SENS	-40	Sensitivities were not initialized.
IDA_SRES_FAIL	-41	The user-provided sensitivity residual function failed in an unrecoverable manner.
IDA_REP_SRES_ERR	-42	The user-provided sensitivity residual function repeatedly returned a recoverable error flag, but the solver was unable to recover.
IDA_BAD_IS	-43	The sensitivity identifier is not valid.
IDA_NO_QUADSENS	-50	Sensitivity-dependent quadratures were not initialized.
IDA_QSRHS_FAIL	-51	The user-provided sensitivity-dependent quadrature right-hand side function failed in an unrecoverable manner.
IDA_FIRST_QSRHS_ERR	-52	The user-provided sensitivity-dependent quadrature right-hand side function failed in an unrecoverable manner on the first call.
IDA_REP_QSRHS_ERR	-53	The user-provided sensitivity-dependent quadrature right-hand side repeatedly returned a recoverable error flag, but the solver was unable to recover.

IDAS **adjoint solver module**		
IDA_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
IDA_NO_FWD	-102	`IDASolveF` has not been previously called.
IDA_NO_BCK	-103	No backward problem was specified.
IDA_BAD_TB0	-104	The desired output for backward problem is outside the interval over which the forward problem was solved.
IDA_REIFWD_FAIL	-105	No checkpoint is available for this hot start.
IDA_FWD_FAIL	-106	`IDASolveB` failed because `IDASolve` was unable to store data between two consecutive checkpoints.
IDA_GETY_BADT	-107	Wrong time in interpolation function.

IDALS **linear solver interface**		
IDALS_SUCCESS	0	Successful function return.
IDALS_MEM_NULL	-1	The `ida_mem` argument was NULL.
IDALS_LMEM_NULL	-2	The IDALS linear solver has not been initialized.
IDALS_ILL_INPUT	-3	The IDALS solver is not compatible with the current NVECTOR module, or an input value was illegal.
IDALS_MEM_FAIL	-4	A memory allocation request failed.
IDALS_PMEM_NULL	-5	The preconditioner module has not been initialized.
IDALS_JACFUNC_UNRECVR	-6	The Jacobian function failed in an unrecoverable manner.
IDALS_JACFUNC_RECVR	-7	The Jacobian function had a recoverable error.
IDALS_SUNMAT_FAIL	-8	An error occurred with the current SUNMATRIX module.
IDALS_SUNLS_FAIL	-9	An error occurred with the current SUNLINSOL module.

IDALS_NO_ADJ   -101   The combined forward-backward problem has not been ini-
                                        tialized.
IDALS_LMEMB_NULL   -102   The linear solver was not initialized for the backward phase.

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

	*continued from last page*
	**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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