User Documentation for CVODES v5.1.0 (SUNDIALS v5.1.0)

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Chapter 1

Introduction

CVODES [49] is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [30]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities. CVODES is a solver for stiff and nonstiff initial value problems (IVPs) for systems of ordinary differential equation (ODEs). In addition to solving stiff and nonstiff ODE systems, CVODES has sensitivity analysis capabilities, using either the forward or the adjoint methods.

1.1 Historical Background

FORTRAN solvers for ODE initial value problems are widespread and heavily used. Two solvers that have been written at LLNL in the past are VODE [8] and VODPK [11]. VODE is a general purpose solver that includes methods for both stiff and nonstiff systems, and in the stiff case uses direct methods (full or banded) for the solution of the linear systems that arise at each implicit step. Externally, VODE is very similar to the well known solver LSODE [45]. VODPK is a variant of VODE that uses a preconditioned Krylov (iterative) method, namely GMRES, for the solution of the linear systems. VODPK is a powerful tool for large stiff systems 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 [9]. The capabilities of both VODE and VODPK have been combined in the C-language package CVODE [16].

At present, CVODE 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) [48], FGMRES (Flexible Generalized Minimum RESidual) [47], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [51], TFQMR (Transpose-Free Quasi-Minimal Residual) [23], and PCG (Preconditioned Conjugate Gradient) [25] linear iterative methods. As Krylov methods, these require almost no matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner matrix, and for most problems preconditioning is essential for an efficient solution. For very large stiff ODE 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-CGStab 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.

In the process of translating the VODE and VODPK algorithms into C, the overall CVODE organization has been changed considerably. One key feature of the CVODE organization is that the linear system solvers comprise a layer of code modules that is separated from the integration algorithm, allowing for easy modification and expansion of the linear solver array. A second key feature is a

separate module devoted to vector operations; this facilitated the extension to multiprosessor environments with minimal impacts on the rest of the solver, resulting in PVODE [13], the parallel variant of CVODE.

CVODES is written with a functionality that is a superset of that of the pair CVODE/PVODE. Sensitivity analysis capabilities, both forward and adjoint, have been added to the main integrator. Enabling forward sensititivity computations in CVODES 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. CVODES provides the infrastructure needed to integrate any final-condition ODE dependent on the solution of the original IVP (in particular the adjoint system).

Development of CVODES was concurrent with a redesign of the vector operations module across the SUNDIALS suite. The key feature of the NVECTOR module is that it is written in terms of abstract vector operations with the actual vector functions attached by a particular implementation (such as serial or parallel) of NVECTOR. This allows writing the SUNDIALS solvers in a manner independent of the actual NVECTOR implementation (which can be user-supplied), as well as allowing more than one NVECTOR module to be linked into an executable file. SUNDIALS (and thus CVODES) is supplied with serial, MPI-parallel, and both OpenMP and Pthreads thread-parallel NVECTOR implementations.

There were several motivations for choosing the C language for CVODE, and later for CVODES. 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. Finally, we prefer C over C++ for CVODES 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.

1.2 Changes from previous versions

Changes in v5.1.0

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

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

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

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

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

Added support for constant damping to the `SUNNonlinearSolver_FixedPoint` module when using Anderson acceleration. See Section 11.4.1 and the `SUNNonlinSolSetDamping_FixedPoint` function for more details.

Changes in v5.0.0

Build system changes

- Increased the minimum required CMake version to 3.5 for most SUNDIALS configurations, and 3.10 when CUDA or OpenMP with device offloading are enabled.

- The CMake option `BLAS_ENABLE` and the variable `BLAS_LIBRARIES` have been removed to simplify builds as SUNDIALS packages do not use BLAS directly. For third party libraries that require linking to BLAS, the path to the BLAS library should be included in the `_LIBRARIES` variable for the third party library *e.g.*, `SUPERLUDIST_LIBRARIES` when enabling SuperLU_DIST.

- Fixed a bug in the build system that prevented the NVECTOR_PTHREADS module from being built.

NVECTOR module changes

- Two new functions were added to aid in creating custom NVECTOR objects. The constructor `N_VNewEmpty` allocates an "empty" generic NVECTOR with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the NVECTOR API by ensuring only required operations need to be set. Additionally, the function `N_VCopyOps(w, v)` has been added to copy the operation function pointers between vector objects. When used in clone routines for custom vector objects these functions also will ease the introduction of any new optional operations to the NVECTOR API by ensuring all operations are copied when cloning objects. See §8.1.5 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 §8.13 and §8.14 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 §8.1.4 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 §8.15 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 §8.9.1 for more details.

- Added new Fortran 2003 interfaces for most NVECTOR modules. See Chapter 8 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 §8.1.5 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 §9.1.2 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 §9.1.1 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 §9.1.3 for more details.

- A new SUNMATRIX (and SUNLINSOL) implementation was added to facilitate the use of the SuperLU_DIST library with SUNDIALS. See §9.6 for more details.

- Added new Fortran 2003 interfaces for most SUNMATRIX modules. See Chapter 9 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 §10.3 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 §10.10 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 §10.12 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 §10.9.2 for more details.

- Added new Fortran 2003 interfaces for most SUNLINSOL modules. See Chapter 10 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 §11.1.8 for more details.

- To facilitate the use of user supplied nonlinear solver convergence test functions the `SUNNonlinSolSetConvTestFn` function in the SUNNONLINSOL API has been updated to take a `void*` data pointer as input. The supplied data pointer will be passed to the nonlinear solver convergence test function on each call.

- The inputs values passed to the first two inputs of the `SUNNonlinSolSolve` function in the SUNNONLINSOL have been changed to be the predicted state and the initial guess for the correction to that state. Additionally, the definitions of `SUNNonlinSolLSetupFn` and `SUNNonlinSolLSolveFn` in the SUNNONLINSOL API have been updated to remove unused input parameters. For more information on the nonlinear system formulation see §11.2 and for more details on the API functions see Chapter 11.

- Added a new SUNNONLINSOL implementation, SUNNONLINSOL_PETSCSNES, which interfaces to the PETSc SNES nonlinear solver API. See §11.5 for more details.

- Added new Fortran 2003 interfaces for most SUNNONLINSOL modules. See Chapter 11 for more details on how to use the interfaces.

CVODES changes

- Fixed a bug in the CVODES constraint handling where the step size could be set below the minimum step size.

- Fixed a bug in the CVODES nonlinear solver interface where the norm of the accumulated correction was not updated when using a non-default convergence test function.

- Fixed a bug in the CVODES `cvRescale` function where the loops to compute the array of scalars for the fused vector scale operation stopped one iteration early.

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

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

- 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, CVODES will remove at least one global reduction per time step.

- The CVLS 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.
- A new linear solver interface function CVLsLinSysFn was added as an alternative method for evaluating the linear system $M = I - \gamma J$.
- Added new functions, CVodeGetCurrentGamma, CVodeGetCurrentState, CVodeGetCurrentStateSens, and CVodeGetCurrentSensSolveIndex which may be useful to users who choose to provide their own nonlinear solver implementations.
- Added a Fortran 2003 interface to CVODES. See Chapter 7 for more details.

Changes in v4.1.0

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

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

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

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

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

Changes in v4.0.2

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

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

Changes in v4.0.1

No changes were made in this release.

Changes in v4.0.0

CVODES' previous direct and iterative linear solver interfaces, CVDLS and CVSPILS, have been merged into a single unified linear solver interface, CVLS, to support any valid SUNLINSOL module. This includes the "DIRECT" and "ITERATIVE" types as well as the new "MATRIX_ITERATIVE" type. Details regarding how CVLS utilizes linear solvers of each type as well as discussion regarding intended use cases for user-supplied SUNLINSOL implementations are included in Chapter 10. All CVODES example programs and the standalone linear solver examples have been updated to use the unified linear solver interface.

The unified interface for the new CVLS module is very similar to the previous CVDLS and CVSPILS 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 CVODES 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 11 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 CVODES example programs have been updated to use generic SUNNONLINSOL modules.

With the introduction of SUNNONLINSOL modules, the input parameter `iter` to `CVodeCreate` has been removed along with the function `CVodeSetIterType` and the constants `CV_NEWTON` and `CV_FUNCTIONAL`. Instead of specifying the nonlinear iteration type when creating the CVODES memory structure, CVODES uses the SUNNONLINSOL_NEWTON module implementation of a Newton iteration by default. For details on using a non-default or user-supplied nonlinear solver see Chapters 4, 5, and 6. CVODES functions for setting the nonlinear solver options (e.g., `CVodeSetMaxNonlinIters`) or getting nonlinear solver statistics (e.g., `CVodeGetNumNonlinSolvIters`) remain unchanged and internally call generic SUNNONLINSOL functions as needed.

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 8 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 §8.11 for more details.

Two changes were made in the CVODE/CVODES/ARKODE initial step size algorithm:

1. Fixed an efficiency bug where an extra call to the right hand side function was made.
2. Changed the behavior of the algorithm if the max-iterations case is hit. Before the algorithm would exit with the step size calculated on the penultimate iteration. Now it will exit with the step size calculated on the final iteration.

Changes in v3.2.1

The changes in this minor release include the following:

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

Changes in v3.2.0

Support for optional inequality constraints on individual components of the solution vector has been added to CVODE and CVODES. See Chapter 2 and the description of `CVodeSetConstraints` in §4.5.7.1 for more details. Use of `CVodeSetConstraints` requires the NVECTOR operations `N_MinQuotient`, `N_VConstrMask`, and `N_VCompare` that were not previously required by CVODE and CVODES.

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

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

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

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

Several changes were made to the build system:

- CMake 3.1.3 is now the minimum required CMake version.
- Deprecate the behavior of the `SUNDIALS_INDEX_TYPE` CMake option and added the `SUNDIALS_INDEX_SIZE` CMake option to select the `sunindextype` integer size.
- The native CMake FindMPI module is now used to locate an MPI installation.

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

Changes in v3.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using rpath by default to locate shared libraries on OSX.
- Fixed Windows specific problem where sunindextype was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows sunindextype is now defined as the MSVC basic type __int64.
- Added sparse SUNMatrix "Reallocate" routine to allow specification of the nonzero storage.
- Updated the KLU SUNLinearSolver module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.
- Updated the "ScaleAdd" and "ScaleAddI" implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum $I + \gamma J$ manually (with zero entries if needed).
- Added new example, cvRoberts_FSA_dns_Switch.c, which demonstrates switching on/off forward sensitivity computations. This example came from the usage notes page of the SUNDIALS website.
- The misnamed function CVSpilsSetJacTimesSetupFnBS has been deprecated and replaced by CVSpilsSetJacTimesBS. The deprecated function CVSpilsSetJacTimesSetupFnBS will be removed in the next major release.
- Changed the LICENSE install path to instdir/include/sundials.

Changes in v3.1.1

The changes in this minor release include the following:

- Fixed a minor bug in the cvSLdet routine, where a return was missing in the error check for three inconsistent roots.

- Fixed a potential memory leak in the SPGMR and SPFGMR linear solvers: if "Initialize" was called multiple times then the solver memory was reallocated (without being freed).
- Updated KLU SUNLINSOL module to use a `typedef` for the precision-specific solve function to be used (to avoid compiler warnings).
- Added missing typecasts for some `(void*)` pointers (again, to avoid compiler warnings).
- Bugfix in `sunmatrix_sparse.c` where we had used `int` instead of `sunindextype` in one location.
- Added missing `#include <stdio.h>` in NVECTOR and SUNMATRIX header files.
- 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 v3.1.0

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

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

Changes in v3.0.0

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

- Added generic SUNMATRIX module with three provided implementations: dense, banded and sparse. These replicate previous SUNDIALS Dls and Sls matrix structures in a single object-oriented API.
- Added example problems demonstrating use of generic SUNMATRIX modules.
- Added generic SUNLINEARSOLVER module with eleven provided implementations: dense, banded, LAPACK dense, LAPACK band, KLU, SuperLU_MT, SPGMR, SPBCGS, SPTFQMR, SPFGMR, PCG. These replicate previous SUNDIALS generic linear solvers in a single object-oriented API.
- Added example problems demonstrating use of generic SUNLINEARSOLVER modules.
- Expanded package-provided direct linear solver (Dls) interfaces and scaled, preconditioned, iterative linear solver (Spils) interfaces to utilize generic SUNMATRIX and SUNLINEARSOLVER objects.
- Removed package-specific, linear solver-specific, solver modules (e.g. CVDENSE, KINBAND, IDAKLU, ARKSPGMR) since their functionality is entirely replicated by the generic Dls/Spils interfaces and SUNLINEARSOLVER/SUNMATRIX modules. The exception is CVDIAG, a diagonal approximate Jacobian solver available to CVODE and CVODES.
- Converted all SUNDIALS example problems to utilize new generic SUNMATRIX and SUNLINEARSOLVER objects, along with updated Dls and Spils linear solver interfaces.

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

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

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

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

In addition, numerous changes were made to the build system. 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 made in `CVodeFree` to call `lfree` unconditionally (if non-NULL).

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

Changes in v2.9.0

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

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

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

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

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

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

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

Changes in v2.8.0

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

Otherwise, only relatively minor modifications were made to the CVODES solver:

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

Some minor changes were made in order to minimize the differences between the sources for private functions in CVODES and CVODE.

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

In `CVodeQuadSensInit`, the line `cv_mem->cv_fQS_data = ...` was corrected (missing `Q`).

In the User Guide, a paragraph was added in Section 6.2.1 on `CVodeAdjReInit`, and a paragraph was added in Section 6.2.9 on `CVodeGetAdjY`. In the example `cvsRoberts_ASAi_dns`, the output was revised to include the use of `CVodeGetAdjY`.

Two minor bugs were fixed regarding the testing of input on the first call to `CVode` – one involving `tstop` and one involving the initialization of `*tret`.

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 example programs.

In the example `cvsHessian_ASA_FSA`, an error was corrected in the function `fB2`: `y2` in place of `y3` in the third term of `Ith(yBdot,6)`.

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

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

Changes in v2.7.0

One significant design change was made with this release: The problem size and its relatives, bandwidth parameters, related internal indices, pivot arrays, and the optional output `lsflag` have all been changed from type `int` to type `long int`, except for the problem size and bandwidths in user

calls to routines specifying BLAS/LAPACK routines for the dense/band linear solvers. The function `NewIntArray` is replaced by a pair `NewIntArray`/`NewLintArray`, for `int` and `long int` arrays, respectively. In a minor change to the user interface, the type of the index `which` in CVODES 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: In `CVSetTqBDF`, the logic was changed to avoid a divide by zero. 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. In the rootfinding functions `CVRcheck1`/`CVRcheck2`, when an exact zero is found, the array `glo` of g values at the left endpoint is adjusted, instead of shifting the t location `tlo` slightly. In the installation files, we modified the treatment of the macro SUNDIALS_USE_GENERIC_MATH, so that the parameter GENERIC_MATH_LIB is either defined (with no value) or not defined.

Changes in v2.6.0

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

This version also includes several new features related to sensitivity analysis, among which are: (a) support for integration of quadrature equations depending on both the states and forward sensitivity (and thus support for forward sensitivity analysis of quadrature equations), (b) support for simultaneous integration of multiple backward problems based on the same underlying ODE (e.g., for use in an *forward-over-adjoint* method for computing second order derivative information), (c) support for backward integration of ODEs and quadratures depending on both forward states and sensitivities (e.g., for use in computing second-order derivative information), and (d) support for reinitialization of the adjoint module.

The user interface has been further refined. Some of the API changes involve: (a) a reorganization of all linear solver modules into two families (besides the existing family of scaled preconditioned iterative linear solvers, the direct solvers, including the new LAPACK-based ones, were also organized into a *direct* family); (b) maintaining a single pointer to user data, optionally specified through a `Set`-type function; and (c) a general streamlining of the preconditioner modules distributed with the solver. Moreover, the prototypes of all functions related to integration of backward problems were modified to support the simultaneous integration of multiple problems. All backward problems defined by the user are internally managed through a linked list and identified in the user interface through a unique identifier.

Changes in v2.5.0

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

In the adjoint solver module, the following two bugs were fixed: in `CVodeF` the solver was sometimes incorrectly taking an additional step before returning control to the user (in `CV_NORMAL` mode) thus leading to a failure in the interpolated output function; in `CVodeB`, while searching for the current check point, the solver was sometimes reaching outside the integration interval resulting in a segmentation fault.

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

Changes in v2.4.0

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

A new interpolation method was added to the CVODES adjoint module. The function `CVadjMalloc` has an additional argument which can be used to select the desired interpolation scheme.

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

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

Changes in v2.3.0

A minor bug was fixed in the interpolation functions of the adjoint CVODES module.

Changes in v2.2.0

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

Changes in v2.1.2

A bug was fixed in the `CVode` function that was potentially leading to erroneous behaviour of the rootfinding procedure on the integration first step.

Changes in v2.1.1

This CVODES release includes bug fixes related to forward sensitivity computations (possible loss of accuray on a BDF order increase and incorrect logic in testing user-supplied absolute tolerances). In addition, we have added the option of activating and deactivating forward sensitivity calculations on successive CVODES runs without memory allocation/deallocation.

Other changes in this minor SUNDIALS release affect the build system.

Changes in v2.1.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the `iopt` and `ropt` arrays. Instead, CVODES now provides a set of routines (with prefix `CVodeSet`) to change the default values for various quantities controlling the solver and a set of extraction routines (with prefix `CVodeGet`) to extract statistics after return from the main solver routine. Similarly, each linear solver module provides its own set of `Set`- and `Get`-type routines. For more details see §4.5.7 and §4.5.9.

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

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

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

1.3 Reading this User Guide

This user guide is a combination of general usage instructions. Specific example programs are provided as a separate document. We expect that some readers will want to concentrate on the general instructions, while others will refer mostly to the examples, and the organization is intended to accommodate both styles.

There are different possible levels of usage of CVODES. The most casual user, with a small IVP problem only, can get by with reading §2.1, then Chapter 4 through §4.5.6 only, and looking at examples in [50]. In addition, to solve a forward sensitivity problem the user should read §2.6, followed by Chapter 5 through §5.2.5 only, and look at examples in [50].

In a different direction, a more expert user with an IVP problem may want to (a) use a package preconditioner (§4.8), (b) supply his/her own Jacobian or preconditioner routines (§4.6), (c) do multiple runs of problems of the same size (§4.5.10), (d) supply a new NVECTOR module (Chapter 8), or even (e) supply new SUNLINSOL and/or SUNMATRIX modules (Chapters 9 and 10). An advanced user with a forward sensitivity problem may also want to (a) provide his/her own sensitivity equations right-hand side routine (§5.3), (b) perform multiple runs with the same number of sensitivity parameters (§5.2.1), or (c) extract additional diagnostic information (§5.2.5). A user with an adjoint sensitivity problem needs to understand the IVP solution approach at the desired level and also go through §2.7 for a short mathematical description of the adjoint approach, Chapter 6 for the usage of the adjoint module in CVODES, and the examples in [50].

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by CVODES for the solution of initial value problems for systems of ODEs, continue with short descriptions of preconditioning (§2.2), stability limit detection (§2.3), and rootfinding (§2.4), and conclude with an overview of the mathematical aspects of sensitivity analysis, both forward (§2.6) and adjoint (§2.7).

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

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

- Chapter 5 describes the usage of CVODES 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 CVODES for adjoint sensitivity analysis. We begin by describing the CVODES 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 8 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, and details on the NVECTOR implementations provided with SUNDIALS.

- Chapter 9 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 (§9.3), a banded implementation (§9.4) and a sparse implementation (§9.5).

- Chapter 10 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.

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

Finally, the reader should be aware of the following notational conventions in this user guide: program listings and identifiers (such as `CVodeInit`) within textual explanations appear in typewriter type style; fields in C structures (such as *content*) appear in italics; and packages or modules, such as CVDLS, 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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1.4.3 SUNDIALS Release Numbers

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Chapter 2

Mathematical Considerations

CVODES solves ODE initial value problems (IVPs) in real N-space, which we write in the abstract form

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

where $y \in \mathbf{R}^N$. Here we use $\dot{y}$ to denote dy/dt. While we use t to denote the independent variable, and usually this is time, it certainly need not be. CVODES solves both stiff and nonstiff systems. Roughly speaking, stiffness is characterized by the presence of at least one rapidly damped mode, whose time constant is small compared to the time scale of the solution itself.

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

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

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

2.1 IVP solution

The methods used in CVODES are variable-order, variable-step multistep methods, based on formulas of the form

$$\sum_{i=0}^{K_1} \alpha_{n,i} y^{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{y}^{n-i} = 0\,. \tag{2.3}$$

Here the y^n are computed approximations to $y(t_n)$, and $h_n = t_n - t_{n-1}$ is the step size. The user of CVODE must choose appropriately one of two multistep methods. For nonstiff problems, CVODE includes the Adams-Moulton formulas, characterized by $K_1 = 1$ and $K_2 = q - 1$ above, where the order q varies between 1 and 12. For stiff problems, CVODES includes the Backward Differentiation Formulas (BDF) in so-called fixed-leading coefficient (FLC) form, given by $K_1 = q$ and $K_2 = 0$, with order q varying between 1 and 5. The coefficients are uniquely determined by the method type, its order, the recent history of the step sizes, and the normalization $\alpha_{n,0} = -1$. See [12] and [35].

For either choice of formula, a nonlinear system must be solved (approximately) at each integration step. This nonlinear system can be formulated as either a rootfinding problem

$$F(y^n) \equiv y^n - h_n \beta_{n,0} f(t_n, y^n) - a_n = 0\,, \tag{2.4}$$

or as a fixed-point problem

$$G(y^n) \equiv h_n \beta_{n,0} f(t_n, y^n) + a_n = y^n\,. \tag{2.5}$$

where $a_n \equiv \sum_{i>0}(\alpha_{n,i} y^{n-i} + h_n \beta_{n,i} \dot{y}^{n-i})$. CVODES provides several nonlinear solver choices as well as the option of using a user-defined nonlinear solver (see Chapter 11). By default CVODES solves (2.4) with a *Newton iteration* which requires the solution of linear systems

$$M[y^{n(m+1)} - y^{n(m)}] = -F(y^{n(m)}), \tag{2.6}$$

in which

$$M \approx I - \gamma J, \quad J = \partial f / \partial y, \quad \text{and} \quad \gamma = h_n \beta_{n,0}. \tag{2.7}$$

The exact variation of the Newton iteration depends on the choice of linear solver and is discussed below and in §11.3. For nonstiff systems, a *fixed-point iteration* (previously referred to as a functional iteration in this guide) for solving (2.5) is also available. This involves evaluations of f only and can (optionally) use Anderson's method [5, 52, 21, 42] to accelerate convergence (see §11.4 for more details). For any nonlinear solver, the initial guess for the iteration is a predicted value $y^{n(0)}$ computed explicitly from the available history data.

For nonlinear solvers that require the solution of the linear system (2.6) (e.g., the default Newton iteration), CVODES provides several linear solver choices, including the option of a user-supplied linear solver module (see Chapter 10). The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices, and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- band direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- sparse direct solver interfaces, using either the KLU sparse solver library [17, 1], or the thread-enabled SuperLU_MT sparse solver library [39, 19, 4] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of CVODES],
- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver,
- SPFGMR, a scaled preconditioned FGMRES (Flexible Generalized Minimal Residual method) solver,
- SPBCGS, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver,
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver, or
- PCG, a scaled preconditioned CG (Conjugate Gradient method) solver.

For large stiff systems, where direct methods are often 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 [9].

In addition, CVODE also provides a linear solver module which only uses a diagonal approximation of the Jacobian matrix.

Note that the dense, band, and sparse direct linear solvers can only be used with the serial and threaded vector representations. The diagonal solver can be used with any vector representation.

In the process of controlling errors at various levels, CVODES 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

$$W_i = 1/[\text{RTOL} \cdot |y_i| + \text{ATOL}_i]. \tag{2.8}$$

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 cases of a matrix-based linear solver, the default Newton iteration is a Modified Newton iteration, in that the iteration matrix M is fixed throughout the nonlinear iterations. However, in the case that a matrix-free iterative linear solver is used, the default Newton iteration is an Inexact Newton iteration, in which M is applied in a matrix-free manner, with matrix-vector products Jv obtained by either difference quotients or a user-supplied routine. With the default Newton iteration, the matrix M 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,
- more than 20 steps have been taken since the last update,
- the value $\bar{\gamma}$ of γ at the last update satisfies $|\gamma/\bar{\gamma} - 1| > 0.3$,
- a non-fatal convergence failure just occurred, or
- an error test failure just occurred.

When forced by a convergence failure, an update of M or P may or may not involve a reevaluation of J (in M) or of Jacobian data (in P), depending on whether Jacobian error was the likely cause of the failure. More generally, the decision is made to reevaluate J (or instruct the user to reevaluate Jacobian data in P) when:

- starting the problem,
- more than 50 steps have been taken since the last evaluation,
- a convergence failure occurred with an outdated matrix, and the value $\bar{\gamma}$ of γ at the last update satisfies $|\gamma/\bar{\gamma} - 1| < 0.2$, or
- a convergence failure occurred that forced a step size reduction.

The default stopping test for nonlinear solver iterations is related to the subsequent local error test, with the goal of keeping the nonlinear iteration errors from interfering with local error control. As described below, the final computed value $y^{n(m)}$ will have to satisfy a local error test $\|y^{n(m)} - y^{n(0)}\| \leq \epsilon$. Letting y^n denote the exact solution of (2.4), we want to ensure that the iteration error $y^n - y^{n(m)}$ is small relative to ϵ, specifically that it is less than 0.1ϵ. (The safety factor 0.1 can be changed by the user.) For this, we also estimate the linear convergence rate constant R as follows. We initialize R to 1, and reset $R = 1$ when M or P is updated. After computing a correction $\delta_m = y^{n(m)} - y^{n(m-1)}$, we update R if $m > 1$ as

$$R \leftarrow \max\{0.3R, \|\delta_m\|/\|\delta_{m-1}\|\}\,.$$

Now we use the estimate

$$\|y^n - y^{n(m)}\| \approx \|y^{n(m+1)} - y^{n(m)}\| \approx R\|y^{n(m)} - y^{n(m-1)}\| = R\|\delta_m\|\,.$$

Therefore the convergence (stopping) test is

$$R\|\delta_m\| < 0.1\epsilon\,.$$

We allow at most 3 iterations (but this limit can be changed by the user). We also declare the iteration diverged if any $\|\delta_m\|/\|\delta_{m-1}\| > 2$ with $m > 1$. If convergence fails with J or P current, we are forced to reduce the step size, and we replace h_n by $h_n/4$. The integration is halted after a preset number of convergence failures; the default value of this limit is 10, but this can be changed by the user.

When an iterative method is used to solve the linear system, its errors must also be controlled, and this also involves the local error test constant. The linear iteration error in the solution vector δ_m is approximated by the preconditioned residual vector. Thus to ensure (or attempt to ensure) that the

linear iteration errors do not interfere with the nonlinear error and local integration error controls, we require that the norm of the preconditioned residual be less than $0.05 \cdot (0.1\epsilon)$.

When the Jacobian is stored using either dense or band SUNMATRIX objects, the Jacobian may be supplied by a user routine, or approximated by difference quotients, at the user's option. In the latter case, we use the usual approximation

$$J_{ij} = [f_i(t, y + \sigma_j e_j) - f_i(t, y)]/\sigma_j \,.$$

The increments σ_j are given by

$$\sigma_j = \max\left\{\sqrt{U}\,|y_j|, \sigma_0/W_j\right\} \,,$$

where U is the unit roundoff, σ_0 is a dimensionless value, and W_j is the error weight defined in (2.8). In the dense case, this scheme requires N evaluations of f, one for each column of J. In the band case, the columns of J are computed in groups, by the Curtis-Powell-Reid algorithm, with the number of f evaluations equal to the bandwidth.

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

In the case of a Krylov method, preconditioning may be used on the left, on the right, or both, with user-supplied routines for the preconditioning setup and solve operations, and optionally also for the required matrix-vector products Jv. If a routine for Jv is not supplied, these products are computed as

$$Jv = [f(t, y + \sigma v) - f(t, y)]/\sigma \,. \tag{2.9}$$

The increment σ is $1/\|v\|$, so that σv has norm 1.

A critical part of CVODES — making it an ODE "solver" rather than just an ODE method, is its control of local error. At every step, the local error is estimated and required to satisfy tolerance conditions, and the step is redone with reduced step size whenever that error test fails. As with any linear multistep method, the local truncation error LTE, at order q and step size h, satisfies an asymptotic relation

$$\text{LTE} = Ch^{q+1}y^{(q+1)} + O(h^{q+2})$$

for some constant C, under mild assumptions on the step sizes. A similar relation holds for the error in the predictor $y^{n(0)}$. These are combined to get a relation

$$\text{LTE} = C'[y^n - y^{n(0)}] + O(h^{q+2}) \,.$$

The local error test is simply $\|\text{LTE}\| \le 1$. Using the above, it is performed on the predictor-corrector difference $\Delta_n \equiv y^{n(m)} - y^{n(0)}$ (with $y^{n(m)}$ the final iterate computed), and takes the form

$$\|\Delta_n\| \le \epsilon \equiv 1/|C'| \,.$$

If this test passes, the step is considered successful. If it fails, the step is rejected and a new step size h' is computed based on the asymptotic behavior of the local error, namely by the equation

$$(h'/h)^{q+1}\|\Delta_n\| = \epsilon/6 \,.$$

Here 1/6 is a safety factor. A new attempt at the step is made, and the error test repeated. If it fails three times, the order q is reset to 1 (if $q > 1$), or the step is restarted from scratch (if $q = 1$). The ratio h'/h is limited above to 0.2 after two error test failures, and limited below to 0.1 after three. After seven failures, CVODES returns to the user with a give-up message.

In addition to adjusting the step size to meet the local error test, CVODE periodically adjusts the order, with the goal of maximizing the step size. The integration starts out at order 1 and varies the order dynamically after that. The basic idea is to pick the order q for which a polynomial of order q best fits the discrete data involved in the multistep method. However, if either a convergence failure or an error test failure occurred on the step just completed, no change in step size or order is done.

At the current order q, selecting a new step size is done exactly as when the error test fails, giving a tentative step size ratio

$$h'/h = (\epsilon/6\|\Delta_n\|)^{1/(q+1)} \equiv \eta_q \,.$$

We consider changing order only after taking $q+1$ steps at order q, and then we consider only orders $q' = q-1$ (if $q > 1$) or $q' = q+1$ (if $q < 5$). The local truncation error at order q' is estimated using the history data. Then a tentative step size ratio is computed on the basis that this error, $\mathrm{LTE}(q')$, behaves asymptotically as $h^{q'+1}$. With safety factors of 1/6 and 1/10 respectively, these ratios are:

$$h'/h = [1/6\|\mathrm{LTE}(q-1)\|]^{1/q} \equiv \eta_{q-1}$$

and

$$h'/h = [1/10\|\mathrm{LTE}(q+1)\|]^{1/(q+2)} \equiv \eta_{q+1} \,.$$

The new order and step size are then set according to

$$\eta = \max\{\eta_{q-1}, \eta_q, \eta_{q+1}\} \;, \quad h' = \eta h \,,$$

with q' set to the index achieving the above maximum. However, if we find that $\eta < 1.5$, we do not bother with the change. Also, h'/h is always limited to 10, except on the first step, when it is limited to 10^4.

The various algorithmic features of CVODES described above, as inherited from VODE and VODPK, are documented in [8, 11, 29]. They are also summarized in [30].

CVODES permits the user to impose optional inequality constraints on individual components of the solution vector y. Any of the following four constraints can be imposed: $y_i > 0$, $y_i < 0$, $y_i \geq 0$, or $y_i \leq 0$. The constraint satisfaction is tested after a successful nonlinear system solution. If any constraint fails, we declare a convergence failure of the Newton iteration and reduce the step size. Rather than cutting the step size by some arbitrary factor, CVODES estimates a new step size h' using a linear approximation ofthe components in y that failed the constraint test (including a afety factor of 0.9 to cover the strict inequality case). If a step fails to satisfy the constraints repeatedly within a step attempt or fails with the minimum step size 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, CVODES takes steps until a user-defined output value $t = t_{\mathrm{out}}$ is overtaken, and then it 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 CVODES 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 the linear system (2.6) (e.g., the default Newton iteration), CVODES makes repeated use of a linear solver to solve linear systems of the form $Mx = -r$, where x is a correction vector and r is a residual vector. 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, as $(P^{-1}A)x = P^{-1}b$; on the right, as $(AP^{-1})Px = b$; or on both sides, as $(P_L^{-1}AP_R^{-1})P_Rx = P_L^{-1}b$. 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. In order to improve the convergence of the Krylov iteration, the preconditioner matrix P, or the product P_LP_R in the last case, should in some sense approximate the system matrix A. Yet at the same time, in order to be cost-effective, the matrix P, or matrices P_L and P_R, 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 [9] for an extensive study of preconditioners for reaction-transport systems).

Most of the iterative linear solvers supplied with SUNDIALS allow for preconditioning either side, or on both sides, although we know of no situation where preconditioning on both sides is clearly

superior to preconditioning on one side only (with the product $P_L P_R$). Moreover, for a given preconditioner matrix, the merits of left vs. right preconditioning are unclear in general, and the user should experiment with both choices. Performance will differ because the inverse of the left preconditioner is included in the linear system residual whose norm is being tested in the Krylov algorithm. As a rule, however, if the preconditioner is the product of two matrices, we recommend that preconditioning be done either on the left only or the right only, rather than using one factor on each side.

Typical preconditioners used with CVODES are based on approximations to the system Jacobian, $J = \partial f/\partial y$. Since the matrix involved is $M = I - \gamma J$, any approximation $\bar{J}$ to J yields a matrix that is of potential use as a preconditioner, namely $P = I - \gamma \bar{J}$. Because the linear solver 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 BDF stability limit detection

CVODES includes an algorithm, STALD (STAbility Limit Detection), which provides protection against potentially unstable behavior of the BDF multistep integration methods in certain situations, as described below.

When the BDF option is selected, CVODES uses Backward Differentiation Formula methods of orders 1 to 5. At order 1 or 2, the BDF method is A-stable, meaning that for any complex constant λ in the open left half-plane, the method is unconditionally stable (for any step size) for the standard scalar model problem $\dot{y} = \lambda y$. For an ODE system, this means that, roughly speaking, as long as all modes in the system are stable, the method is also stable for any choice of step size, at least in the sense of a local linear stability analysis.

At orders 3 to 5, the BDF methods are not A-stable, although they are *stiffly stable*. In each case, in order for the method to be stable at step size h on the scalar model problem, the product $h\lambda$ must lie within a *region of absolute stability*. That region excludes a portion of the left half-plane that is concentrated near the imaginary axis. The size of that region of instability grows as the order increases from 3 to 5. What this means is that, when running BDF at any of these orders, if an eigenvalue λ of the system lies close enough to the imaginary axis, the step sizes h for which the method is stable are limited (at least according to the linear stability theory) to a set that prevents $h\lambda$ from leaving the stability region. The meaning of *close enough* depends on the order. At order 3, the unstable region is much narrower than at order 5, so the potential for unstable behavior grows with order.

System eigenvalues that are likely to run into this instability are ones that correspond to weakly damped oscillations. A pure undamped oscillation corresponds to an eigenvalue on the imaginary axis. Problems with modes of that kind call for different considerations, since the oscillation generally must be followed by the solver, and this requires step sizes ($h \sim 1/\nu$, where ν is the frequency) that are stable for BDF anyway. But for a weakly damped oscillatory mode, the oscillation in the solution is eventually damped to the noise level, and at that time it is important that the solver not be restricted to step sizes on the order of $1/\nu$. It is in this situation that the new option may be of great value.

In terms of partial differential equations, the typical problems for which the stability limit detection option is appropriate are ODE systems resulting from semi-discretized PDEs (i.e., PDEs discretized in space) with advection and diffusion, but with advection dominating over diffusion. Diffusion alone produces pure decay modes, while advection tends to produce undamped oscillatory modes. A mix of the two with advection dominant will have weakly damped oscillatory modes.

The STALD algorithm attempts to detect, in a direct manner, the presence of a stability region boundary that is limiting the step sizes in the presence of a weakly damped oscillation [27]. The algorithm supplements (but differs greatly from) the existing algorithms in CVODES for choosing step size and order based on estimated local truncation errors. The STALD algorithm works directly with

history data that is readily available in CVODES. If it concludes that the step size is in fact stability-limited, it dictates a reduction in the method order, regardless of the outcome of the error-based algorithm. The STALD algorithm has been tested in combination with the VODE solver on linear advection-dominated advection-diffusion problems [28], where it works well. The implementation in CVODES has been successfully tested on linear and nonlinear advection-diffusion problems, among others.

This stability limit detection option adds some computational overhead to the CVODES solution. (In timing tests, these overhead costs have ranged from 2% to 7% of the total, depending on the size and complexity of the problem, with lower relative costs for larger problems.) Therefore, it should be activated only when there is reasonable expectation of modes in the user's system for which it is appropriate. In particular, if a CVODE solution with this option turned off appears to take an inordinately large number of steps at orders 3-5 for no apparent reason in terms of the solution time scale, then there is a good chance that step sizes are being limited by stability, and that turning on the option will improve the efficiency of the solution.

2.4 Rootfinding

The CVODES solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (2.1), CVODES can also find the roots of a set of user-defined functions $g_i(t, y)$ that depend both on t and on the solution vector $y = y(t)$. 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 $g_i(t, y(t))$, 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 CVODES. 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 hone in on the root(s) with a modified secant method [26]. In addition, each time g is computed, CVODES 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, CVODES 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, CVODES stops and reports an error. This way, each time CVODES 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, CVODES 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}, 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_i at t_{hi} for zeros and for sign changes in (t_{lo}, t_{hi}). If no sign changes were 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 include 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 is 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 $\tau/2$.

2.5 Pure quadrature integration

In many applications, and most notably during the backward integration phase of an adjoint sensitivity analysis run (see §2.7) it is of interest to compute integral quantities of the form

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

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):

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

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 CVODES the extended ODE 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 ODE. Moreover, since the additional states z do not enter the right-hand side of the ODE (2.10) and therefore the right-hand side of the extended ODE system, it is much more efficient to treat the ODE system (2.10) separately from the original 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

$$z^n = -\frac{1}{\alpha_{n,0}} \left(h_n \beta_{n,0} q(t_n, y_n, p) + h_n \sum_{i=1}^{K_2} \beta_{n,i} \dot{z}^{n-i} + \sum_{i=1}^{K_1} \alpha_{n,i} z^{n-i} \right) \ ,$$

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.

2.6 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 ODEs, 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):

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

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

When performing forward sensitivity analysis, CVODES carries out the time integration of the combined system, (2.2) and (2.12), by viewing it as an ODE 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 ODEs. In particular, for stiff systems, for which CVODES employs a Newton iteration, the original ODE system and all sensitivity systems share the same Jacobian matrix, and therefore the same iteration matrix M in (2.7).

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

2.6.1 Forward sensitivity methods

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

- *Staggered Direct*

  In this approach [15], 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 or Adams) 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 M in (2.7), it must be updated and factored at every step of the integration, in contrast to an evalutaion of M 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 [38]. 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 CVODES.

- *Simultaneous Corrector*

  In this method [43], the discretization is applied simultaneously to both the original equations (2.2) and the sensitivity systems (2.12) resulting in the following nonlinear system

  $$\hat{F}(\hat{y}_n) \equiv \hat{y}_n - h_n \beta_{n,0} \hat{f}(t_n, \hat{y}_n) - \hat{a}_n = 0\,,$$

  where $\hat{f} = [f(t, y, p), \ldots, (\partial f/\partial y)(t, y, p)s_i + (\partial f/\partial p_i)(t, y, p), \ldots]$, and $\hat{a}_n$ is comprised of the terms in the discretization that depend on the solution at previous integration steps. This combined nonlinear system can be solved using a modified Newton method as in (2.6) by solving the corrector equation

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

  at each iteration, where

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

  M is defined as in (2.7), and $J_i = (\partial/\partial y)\,[(\partial f/\partial y)s_i + (\partial f/\partial p_i)]$. It can be shown that 2-step quadratic convergence can be retained by using only the block-diagonal portion of $\hat{M}$ in the corrector equation (2.13). This results in a decoupling that allows the reuse of M without additional matrix factorizations. However, the products $(\partial f/\partial y)s_i$ and the vectors $\partial f/\partial p_i$ must still be reevaluated at each step of the iterative process (2.13) to update the sensitivity portions of the residual $\hat{G}$.

- *Staggered corrector*

  In this approach [22], as in the staggered direct method, the nonlinear system (2.4) is solved first using the Newton iteration (2.6). Then a separate Newton iteration is used to solve the sensitivity system (2.12):

$$M[s_i^{n(m+1)} - s_i^{n(m)}] = \\ -\left[s_i^{n(m)} - \gamma\left(\frac{\partial f}{\partial y}(t_n, y^n, p)s_i^{n(m)} + \frac{\partial f}{\partial p_i}(t_n, y^n, p)\right) - a_{i,n}\right], \quad (2.14)$$

  where $a_{i,n} = \sum_{j>0}(\alpha_{n,j}s_i^{n-j} + h_n\beta_{n,j}\dot{s}_i^{n-j})$. In other words, a modified Newton iteration is used to solve a linear system. In this approach, the vectors $\partial f/\partial p_i$ need be updated only once per integration step, after the state correction phase (2.6) has converged. Note also that Jacobian-related data can be reused at all iterations (2.14) to evaluate the products $(\partial f/\partial y)s_i$.

CVODES implements the simultaneous corrector method and two flavors of the staggered corrector method which differ only if the sensitivity variables are included in the error control test. In the *full error control* case, the first variant of the staggered corrector method requires the convergence of the iterations (2.14) for all N_s sensitivity systems and then performs the error test on the sensitivity variables. The second variant of the method will perform the error test for each sensitivity vector $s_i, (i = 1, 2, \ldots, N_s)$ individually, as they pass the convergence test. Differences in performance between the two variants may therefore be noticed whenever one of the sensitivity vectors s_i fails a convergence or error test.

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 M 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.

2.6.2 Selection of the absolute tolerances for sensitivity variables

If the sensitivities are included in the error test, CVODES 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 CVODES can provide different values as an option.

2.6.3 Evaluation of the sensitivity right-hand side

There are several methods for evaluating the right-hand side of the sensitivity systems (2.12): analytic evaluation, automatic differentiation, complex-step approximation, and finite differences (or directional derivatives). CVODES 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), CVODES can evaluate these quantities using various finite difference-based approximations to evaluate the terms $(\partial f/\partial y)s_i$ and $(\partial f/\partial p_i)$, or using directional derivatives to evaluate $[(\partial f/\partial y)s_i + (\partial f/\partial p_i)]$. As is typical for finite differences, the proper choice of perturbations is a delicate matter. CVODES takes into account several problem-related features: the

relative ODE 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 $(\partial f/\partial y)s_i$ and $\partial f/\partial p_i$ in the right-hand side of (2.12) can be evaluated either separately:

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

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

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

or simultaneously:

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

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

or by adaptively switching between (2.15)+(2.15') and (2.16), depending on the relative size of the 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 finite difference and directional derivative formulas have also been implemented for one-sided difference formulas. Forward finite differences can be applied to $(\partial f/\partial y)s_i$ and $\partial f/\partial p_i$ separately, or the single directional derivative formula

$$\frac{\partial f}{\partial y} s_i + \frac{\partial f}{\partial p_i} \approx \frac{f(t, y+\sigma s_i, p+\sigma e_i) - f(t, y, p)}{\sigma}$$

can be used. In CVODES, 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.

2.6.4 Quadratures depending on forward sensitivities

If pure quadrature variables are also included in the problem definition (see §2.5), CVODES 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, CVODES provides support for computing integrals of the form:

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

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

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

as integrands for $\bar{z}$, where q_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.

2.7 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 ODE 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. 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 [14]. Introducing a Lagrange multiplier λ, we form the augmented objective function

$$I(p) = G(p) - \int_{t_0}^{T} \lambda^* \left(\dot{y} - f(t, y, p)\right) dt\,, \tag{2.18}$$

where $*$ denotes the conjugate transpose. The gradient of G with respect to p is

$$\frac{dG}{dp} = \frac{dI}{dp} = \int_{t_0}^{T} (g_p + g_y s)dt - \int_{t_0}^{T} \lambda^* \left(\dot{s} - f_y s - f_p\right) dt\,, \tag{2.19}$$

where subscripts on functions f or g are used to denote partial derivatives and $s = [s_1, \ldots, s_{N_s}]$ is the matrix of solution sensitivities. Applying integration by parts to the term $\lambda^* \dot{s}$, and by requiring that λ satisfy

$$\begin{aligned} \dot{\lambda} &= -\left(\frac{\partial f}{\partial y}\right)^* \lambda - \left(\frac{\partial g}{\partial y}\right)^* \\ \lambda(T) &= 0\,, \end{aligned} \tag{2.20}$$

the gradient of G with respect to p is nothing but

$$\frac{dG}{dp} = \lambda^*(t_0)s(t_0) + \int_{t_0}^{T} \left(g_p + \lambda^* f_p\right) dt\,. \tag{2.21}$$

The gradient of $g(T, y, p)$ with respect to p can be then obtained by using the Leibnitz differentiation rule. Indeed, from (2.17),

$$\frac{dg}{dp}(T) = \frac{d}{dT}\frac{dG}{dp}$$

and therefore, taking into account that dG/dp in (2.21) depends on T both through the upper integration limit and through λ, and that $\lambda(T) = 0$,

$$\frac{dg}{dp}(T) = \mu^*(t_0)s(t_0) + g_p(T) + \int_{t_0}^{T} \mu^* f_p dt\,, \tag{2.22}$$

where μ is the sensitivity of λ with respect to the final integration limit T. Thus μ satisfies the following equation, obtained by taking the total derivative with respect to T of (2.20):

$$\begin{aligned} \dot{\mu} &= -\left(\frac{\partial f}{\partial y}\right)^* \mu \\ \mu(T) &= \left(\frac{\partial g}{\partial y}\right)^*_{t=T}\,. \end{aligned} \tag{2.23}$$

The final condition on $\mu(T)$ follows from $(\partial\lambda/\partial t) + (\partial\lambda/\partial T) = 0$ at T, and therefore, $\mu(T) = -\dot{\lambda}(T)$.

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 same holds true for the system (2.23) and the formula (2.22) for gradients of $g(T, y, p)$. The second important remark is that the adjoint systems (2.20) and (2.23) are terminal value problems which depend 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 CVODES during the backward integration phase of (2.20) or (2.23). The approach adopted in CVODES, based on *checkpointing*, is described below.

2.7.1 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 CVODES 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 CVODES 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. CVODES 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, CVODES settles for a compromise between storage space and execution time by implementing a so-called *checkpointing scheme*. At the cost of at most one additional forward integration, this approach offers the best possible estimate of memory requirements for adjoint sensitivity analysis. To begin with, based on the problem size N and the available memory, the user decides on the number N_d of data pairs $(y, \dot{y})$ if cubic Hermite interpolation is selected, or on the number N_d of y vectors in the case of variable-degree polynomial interpolation, that can be kept in memory for the purpose of interpolation. Then, during the first forward integration stage, after every N_d integration steps a checkpoint is formed by saving enough information (either in memory or on disk) to allow for a hot restart, that is a restart which will exactly reproduce the forward integration. In order to avoid storing Jacobian-related data at each checkpoint, a reevaluation of the iteration matrix is forced before each checkpoint. At the end of this stage, we are left with N_c checkpoints, including one at t_0. During the backward integration stage, the adjoint variables are integrated 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] (see Fig. 2.1).

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, CVODES 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).

[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. The accuracy differences are minor when using BDF (since the maximum method order cannot exceed 5), but can be significant for the Adams method for which the order can reach 12.

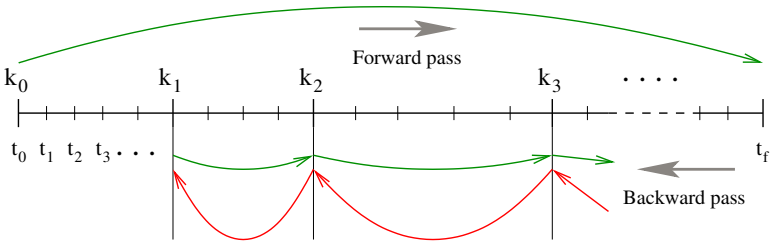

Figure 2.1: Illustration of the checkpointing algorithm for generation of the forward solution during the integration of the adjoint system.

Finally, we note that the adjoint sensitivity module in CVODES provides the necessary infrastructure to integrate backwards in time any ODE terminal value problem dependent on the solution of the IVP (2.2), including adjoint systems (2.20) or (2.23), as well as any other quadrature ODEs that may be needed in evaluating the integrals in (2.21) or (2.22). In particular, for ODE 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.

2.8 Second-order sensitivity analysis

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

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

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

$$\begin{aligned} \dot{y}_{pp} &= \left(f_y \otimes I_{N_p}\right) \cdot y_{pp} + \left(I_N \otimes y_p^T\right) \cdot f_{yy} y_p \\ y_{pp}(t_0) &= \frac{\partial^2 y_0}{\partial p^2} \,, \end{aligned}$$

where y_p is 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 ODE systems of the same dimension N 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 one of the gradients of (2.21) or (2.22). 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. Consider for example, $G(p) = \int_{t_0}^{t_f} g(t, y)\, dt$. 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

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

[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 ODE (2.2) on the parameters p is through its initial conditions only. For details on the derivation in the general case, see [44].

where λ, μ, and s are solutions of

$$\begin{aligned} -\dot{\mu} &= f_y^T \mu + \left(\lambda^T \otimes I_n\right) f_{yy} s + g_{yy} s\,; \quad \mu(t_f) = 0 \\ -\dot{\lambda} &= f_y^T \lambda + g_y^T\,; \quad \lambda(t_f) = 0 \\ \dot{s} &= f_y s\,; \quad s(t_0) = y_{0p} u \end{aligned} \tag{2.24}$$

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, the cost of computing the Hessian-vector product is roughly that of two forward and two backward integrations of a system of ODEs of size N. For more details, including the corresponding formulas for a pointwise model functional output, see [44].

To allow the *foward-over-adjoint* approach described above, CVODES 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).

Chapter 3

Code Organization

3.1 SUNDIALS organization

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

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Figures 3.1 and 3.2). The

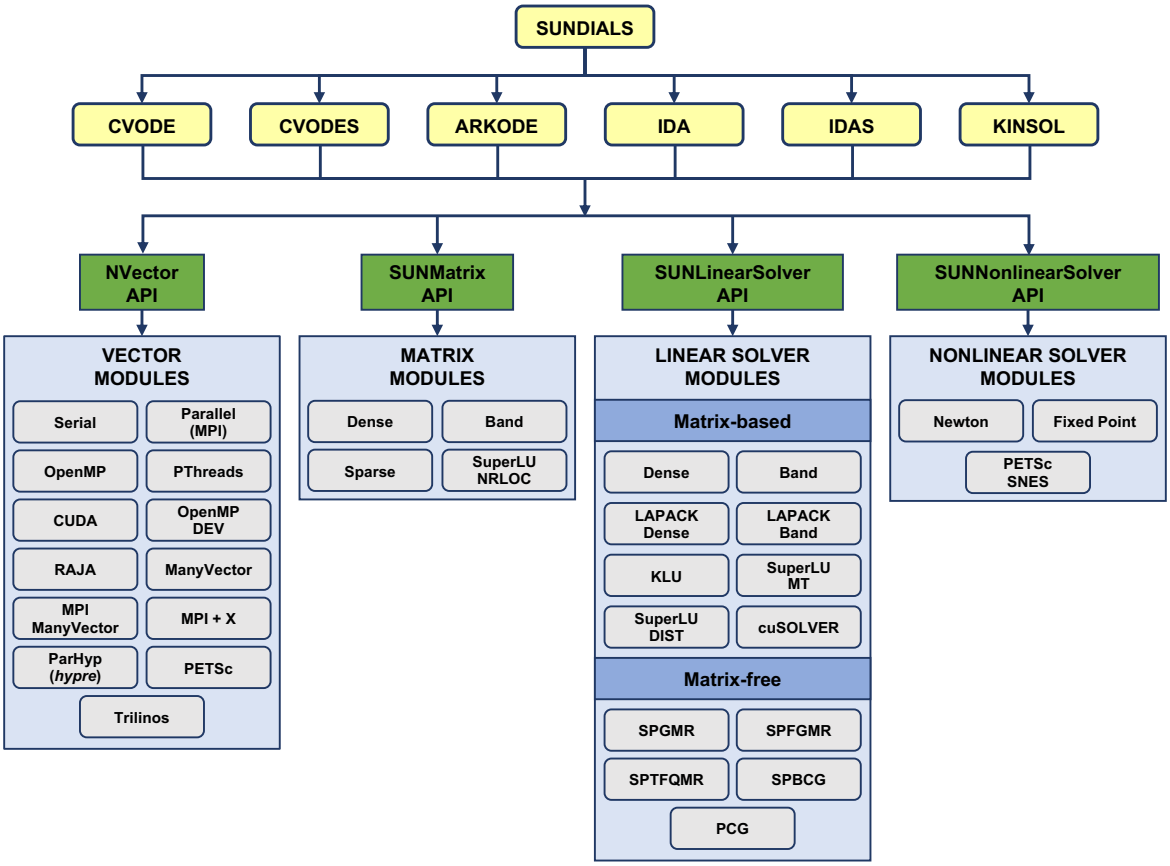

Figure 3.1: High-level diagram of the SUNDIALS suite.

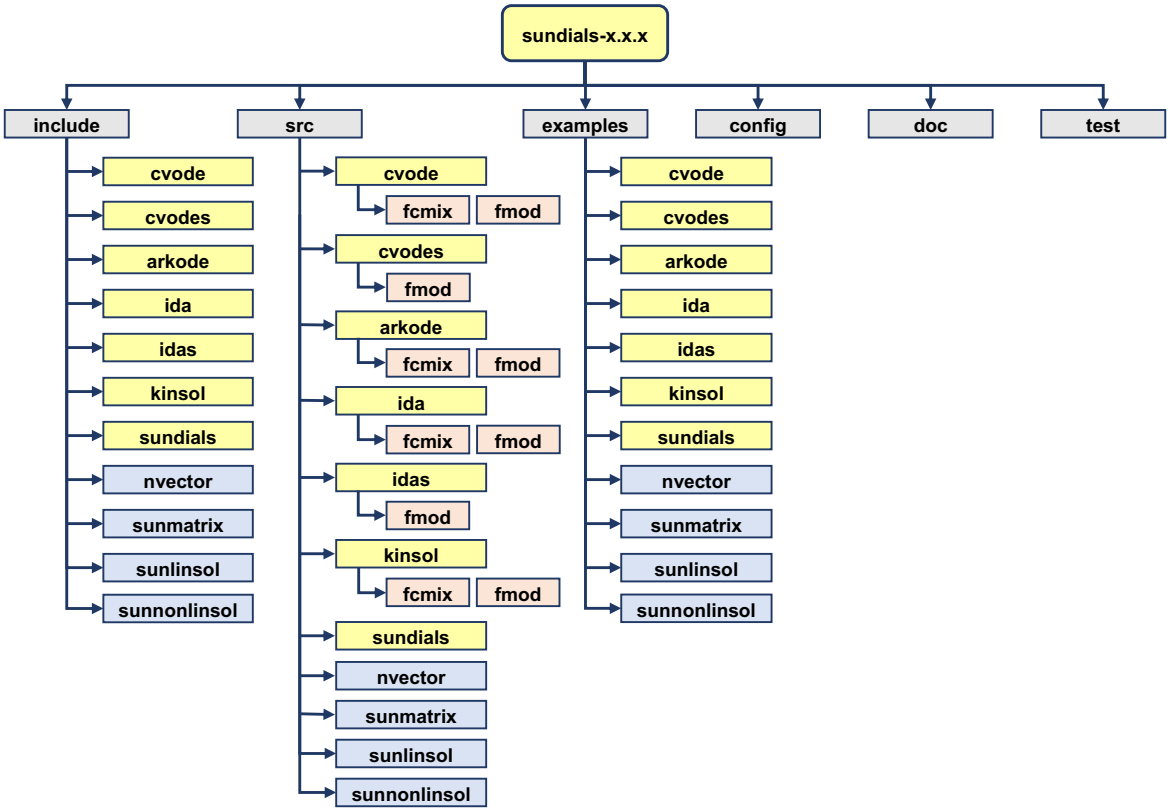

Figure 3.2: Directory structure of the SUNDIALS source tree.

following is a list of the solver packages presently available, and the basic functionality of each:

- CVODE, a solver for stiff and nonstiff ODE systems $dy/dt = f(t, y)$ based on Adams and BDF methods;
- CVODES, a solver for stiff and nonstiff ODE systems with sensitivity analysis capabilities;
- ARKODE, a solver for stiff, nonstiff, mixed stiff-nonstiff, and multirate ODE systems $M dy/dt = f_1(t, y) + f_2(t, y)$ based on Runge-Kutta methods;
- IDA, a solver for differential-algebraic systems $F(t, y, \dot{y}) = 0$ based on BDF methods;
- IDAS, a solver for differential-algebraic systems with sensitivity analysis capabilities;
- KINSOL, a solver for nonlinear algebraic systems $F(u) = 0$.

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

3.2 CVODES organization

The CVODES package is written in ANSI C. 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 CVODES package is shown in Figure 3.3. The basic elements of the structure are a module for the basic integration algorithm (including forward sensitivity analysis), a module for adjoint sensitivity analysis, and support for the solution of nonlinear and linear systems

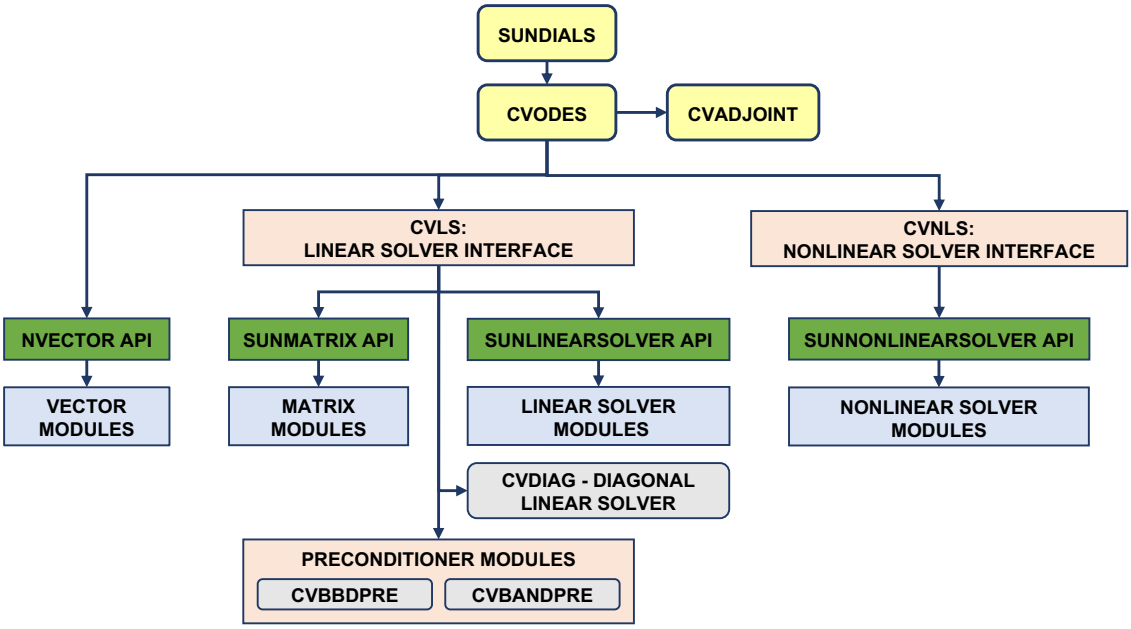

Figure 3.3: Overall structure diagram of the CVODES package. Modules specific to CVODES begin with "CV" (CVLS, CVNLS, CVDIAG, CVBBDPRE, and CVBANDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver modules (see Figure 3.1).

that arise in the case of a stiff system. The central integration module, implemented in the files `cvode.h`, `cvode_impl.h`, and `cvode.c`, deals with the evaluation of integration coefficients, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues.

CVODES utilizes generic linear and nonlinear solver modules defined by the SUNLINSOL API (see Chapter 10) and SUNNONLINSOL API (see Chapter 11), respectively. As such, CVODES has no knowledge of the method being used to solve the linear and nonlinear systems that arise. 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.

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. CVODES provides three different strategies for dealing with the correction stage for the sensitivity variables: `CV_SIMULTANEOUS`, `CV_STAGGERED` and `CV_STAGGERED1` (see §2.6 and §5.2.1). The CVODES package includes an algorithm for the approximation of the sensitivity equations right-hand sides by difference quotients, but the user has the option of supplying these right-hand sides directly.

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

At present, the package includes two linear solver interfaces. The primary linear solver interface, CVLS, supports both direct and iterative linear solvers built using the generic SUNLINSOL API (see Chapter 10). These solvers may utilize a SUNMATRIX object (see Chapter 9) for storing Jacobian information, or they may be matrix-free. Since CVODES can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to CVODES will expand as new SUNLINSOL modules are developed.

Additionally, CVODES includes the *diagonal* linear solver interface, CVDIAG, that creates an inter-

nally generated diagonal approximation to the Jacobian.

For users employing dense or banded Jacobian matrices, CVODES includes algorithms for their approximation through difference quotients, although the user also has the option of supplying a routine to compute 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, CVODES includes an algorithm for the approximation by difference quotients of the product Mv. 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 [9, 11], together with the example and demonstration programs included with CVODES, offer considerable assistance in building preconditioners.

CVODES' linear solver interface consists of four primary phases, 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, and only as required to achieve convergence.

CVODES also provides two preconditioner modules, for use with any of the Krylov iterative linear solvers. The first one, CVBANDPRE, is intended to be used with NVECTOR_SERIAL, NVECTOR_OPENMP or NVECTOR_PTHREADS and provides a banded difference-quotient Jacobian-based preconditioner, with corresponding setup and solve routines. The second preconditioner module, CVBBDPRE, 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 CVODES 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 CVODES 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 CVODES memory structure. The reentrancy of CVODES was motivated by the anticipated multicomputer extension, but is also essential in a uniprocessor setting where two or more problems are solved by intermixed calls to the package from within a single user program.

Chapter 4

Using CVODES for IVP Solution

This chapter is concerned with the use of CVODES for the solution of initial value problems (IVPs) in a C language setting. The following sections treat the header files and the layout of the user's main program, and provide descriptions of the CVODES user-callable functions and user-supplied functions. This usage is essentially equivalent to using CVODE [31].

The sample programs described in the companion document [50] may also be helpful. Those codes may be used as templates (with the removal of some lines used in testing) and are included in the CVODES package.

The user should be aware that not all SUNLINSOL and SUNMATRIX modules are compatible with all NVECTOR implementations. Details on compatibility are given in the documentation for each SUNMATRIX module (Chapter 9) and each SUNLINSOL module (Chapter 10). 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 9 and 10 to verify compatibility between these modules. In addition to that documentation, we note that the CVBANDPRE preconditioning module is only compatible with the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector implementations, and the preconditioner module CVBBDPRE 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.

CVODES 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 CVODES, 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 CVODES. The relevant library files are

- *libdir*/`libsundials_cvodes.`*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/cvodes`
- *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 CVODE and CVODES libraries because both contain user-callable functions with the same names (to ensure that CVODES is backward compatible with CVODE). Therefore, applications that contain both ODE problems and ODEs with sensitivity analysis, should use CVODES.

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:

- `cvodes/cvodes.h`, the main header file for CVODES, which defines the several types and various constants, and includes function prototypes. This includes the header file for CVLS, `cvodes/cvodes_ls.h`.

Note that `cvodes.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 8 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 11 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 (2.6) (e.g., the default Newton iteration), then a linear solver module header file will be required. The header files corresponding to the various SUNDIALS-provided linear solver modules available for use with CVODES are:

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

  - `sunlinsol/sunlinsol_superlumt.h`, which is used with the SUPERLUMT sparse linear solver module, SUNLINSOL_SUPERLUMT;

- Iterative linear solvers:

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

- `cvodes/cvodes_diag.h`, which is used with the CVDIAG diagonal linear solver module.

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 `cvsDiurnal_kry_p` example (see [50]), 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 an ODE IVP. Most of the steps are independent of the NVECTOR, SUNMATRIX, SUNLINSOL, and SUNNONLINSOL implementations used. For the steps that are not, refer to Chapters 8, 9, 10, and 11 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 vector of initial values**

   To set the vector `y0` of initial values, 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 §8.3-8.6 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 §8.7 and §8.8 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 §8.9-8.10 for details.

4. **Create CVODES object**

   Call `cvode_mem = CVodeCreate(lmm)` to create the CVODES memory block and to specify the linear multistep method. `CVodeCreate` returns a pointer to the CVODES memory structure. See §4.5.1 for details.

5. **Initialize CVODES solver**

   Call `CVodeInit(...)` to provide required problem specifications, allocate internal memory for CVODES, and initialize CVODES. `CVodeInit` returns a flag, the value of which indicates either success or an illegal argument value. See §4.5.1 for details.

6. **Specify integration tolerances**

   Call `CVodeSStolerances(...)` or `CVodeSVtolerances(...)` to specify either a scalar relative tolerance and scalar absolute tolerance, or a scalar relative tolerance and a vector of absolute tolerances, respectively. Alternatively, call `CVodeWFtolerances` 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 solve will be used (e.g., the 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 10.

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 10 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 CVLS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with the call (for details see §4.5.3):

    ```
    ier = CVodeSetLinearSolver(...);
    ```

    Alternately, if the CVODES-specific diagonal linear solver module, CVDIAG, is desired, initialize the linear solver module and attach it to CVODES with the call

    ```
    ier = CVDiag(...);
    ```

11. **Set optional inputs**

    Call `CVodeSet*` functions to change any optional inputs that control the behavior of CVODES from their default values. See §4.5.7.1 and §4.5.7 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 11 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 = CVodeSetNonlinearSolver(cvode_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 `CVodeInit` if using the default nonlinear solver or after attaching a new nonlinear solver to CVODE, otherwise the optional inputs will be overridden by CVODES defaults. See Chapter 11 for more information on optional inputs.

15. **Specify rootfinding problem**

    Optionally, call `CVodeRootInit` to initialize a rootfinding problem to be solved during the integration of the ODE system. See §4.5.5, and see §4.5.7.3 for relevant optional input calls.

16. **Advance solution in time**

    For each point at which output is desired, call `ier = CVode(cvode_mem, tout, yout, &tret, itask)`. Here `itask` specifies the return mode. The vector `yout` (which can be the same as the vector `y0` above) will contain $y(t)$. See §4.5.6 for details.

17. **Get optional outputs**

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

18. **Deallocate memory for solution vector**

    Upon completion of the integration, deallocate memory for the vector `y` (or `yout`) by calling the appropriate destructor function defined by the NVECTOR implementation:

    ```
    N_VDestroy(y);
    ```

19. **Free solver memory**

    Call `CVodeFree(&cvode_mem)` to free the memory allocated by CVODES.

20. **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.

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

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

22. **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 10 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 CVODES functions that are called by the user to setup and then solve an IVP. Some of these are required. However, starting with §4.5.7, the functions listed involve optional inputs/outputs or restarting, and those paragraphs may be skipped for a casual use of CVODES. In any case, refer to §4.4 for the correct order of these calls.

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

4.5.1 CVODES 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 IVP solution is complete, as it frees the CVODES memory block created and allocated by the first two calls.

`CVodeCreate`

Call `cvode_mem = CVodeCreate(lmm);`

Description The function `CVodeCreate` instantiates a CVODES solver object and specifies the solution method.

Arguments `lmm` (`int`) specifies the linear multistep method and must be one of two possible values: `CV_ADAMS` or `CV_BDF`.

The recommended choices for `lmm` are `CV_ADAMS` for nonstiff problems and `CV_BDF` for stiff problems. The default Newton iteration is recommended for stiff problems, and the fixed-point solver (previously referred to as the functional iteration in this guide) is recommended for nonstiff problems. For details on how to attach a different nonlinear solver module to CVODES see the description of `CVodeSetNonlinearSolver`.

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

F2003 Name `FCVodeCreate`

`CVodeInit`

Call `flag = CVodeInit(cvode_mem, f, t0, y0);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `f` (`CVRhsFn`) is the C function which computes the right-hand side function f in the ODE. This function has the form `f(t, y, ydot, 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.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeInit` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_MEM_FAIL` A memory allocation request has failed.
- `CV_ILL_INPUT` An input argument to `CVodeInit` has an illegal value.

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

F2003 Name `FCVodeInit`

`CVodeFree`

Call `CVodeFree(&cvode_mem);`

Description The function `CVodeFree` frees the memory allocated by a previous call to `CVodeCreate`.

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

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

F2003 Name `FCVodeFree`

4.5.2 CVODES 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 `CVodeInit`.

`CVodeSStolerances`

Call `flag = CVodeSStolerances(cvode_mem, reltol, abstol);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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:
- `CV_SUCCESS` The call to `CVodeSStolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_MALLOC` The allocation function `CVodeInit` has not been called.
- `CV_ILL_INPUT` One of the input tolerances was negative.

F2003 Name `FCVodeSStolerances`

`CVodeSVtolerances`

Call `flag = CVodeSVtolerances(cvode_mem, reltol, abstol);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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:
- `CV_SUCCESS` The call to `CVodeSVtolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_MALLOC` The allocation function `CVodeInit` has not been called.
- `CV_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 `FCVodeSVtolerances`

`CVodeWFtolerances`

Call `flag = CVodeWFtolerances(cvode_mem, efun);`

Description The function `CVodeWFtolerances` 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. (2.8).

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
`efun` (`CVEwtFn`) 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:

`CV_SUCCESS`	The call to `CVodeWFtolerances` was successful.
`CV_MEM_NULL`	The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
`CV_NO_MALLOC`	The allocation function `CVodeInit` has not been called.

F2003 Name `FCVodeWFtolerances`

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 1.0E-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 `cvsRoberts_dns` in the CVODES package, and the discussion of it in the CVODES Examples document [50]. In that problem, the three components vary betwen 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 some 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 `y` returned by CVODES, with magnitude comparable to `abstol` or less, is equivalent to zero as far as the computation is concerned.

(3) The user's right-hand side routine `f` should never change a negative value in the solution vector `y` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `f` 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 y vector) for the purposes of computing $f(t, y)$.

(4) Positivity and non-negativity constraints on components can be enforced by use of the recoverable error return feature in the user-supplied right-hand side function. However, because this option involves some extra overhead cost, it 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 (2.6) (e.g., the default Newton iteration), there are two CVODES linear solver interfaces currently available for this task: CVLS and CVDIAG.

The first corresponds to the main linear solver interface in CVODES, that supports all valid SUNLINSOL modules. Here, matrix-based SUNLINSOL modules utilize SUNMATRIX objects to store the approximate Jacobian matrix $J = \partial f/\partial y$, the Newton matrix $M = I - \gamma J$, and factorizations used throughout the solution process. Conversely, matrix-free SUNLINSOL modules instead use iterative methods to solve the Newton systems of equations, and only require the *action* of the matrix on a vector, Mv. With most of these methods, preconditioning can be done on the left only, the right only, on both the left and right, or not at all. The exceptions to this rule are SPFGMR that supports right preconditioning only and PCG that performs symmetric preconditioning. For the specification of a preconditioner, see the iterative linear solver sections in §4.5.7 and §4.6.

If preconditioning is done, user-supplied functions define linear operators corresponding to left and right preconditioner matrices P_1 and P_2 (either of which could be the identity matrix), such that the product $P_1 P_2$ approximates the matrix $M = I - \gamma J$ of (2.7).

The CVDIAG linear solver is also a direct linear solver, but it only uses a diagonal approximation to J.

To specify a generic linear solver to CVODES, after the call to `CVodeCreate` but before any calls to `CVodes`, the user's program must create the appropriate `SUNLinearSolver` object and call the function `CVodeSetLinearSolver`, 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 9 and 10.

Once this solver object has been constructed, the user should attach it to CVODES via a call to `CVodeSetLinearSolver`. The first argument passed to this function is the CVODES memory pointer returned by `CVodeCreate`; the second argument is the desired SUNLINSOL object to use for solving linear 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 CVLS linear solver interface, linking it to the main CVODES integrator, and allows the user to specify additional parameters and routines pertinent to their choice of linear solver.

To instead specify the CVODES-specific diagonal linear solver interface, the user's program must call `CVDiag`, as documented below. The first argument passed to this function is the CVODES memory pointer returned by `CVodeCreate`.

`CVodeSetLinearSolver`

Call `flag = CVodeSetLinearSolver(cvode_mem, LS, J);`

Description The function `CVodeSetLinearSolver` attaches a generic SUNLINSOL object `LS` and corresponding template Jacobian SUNMATRIX object `J` to CVODES, initializing the CVLS linear solver interface.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `LS` (`SUNLinearSolver`) SUNLINSOL object to use for solving linear systems of the form (2.6).
- `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

- `CVLS_SUCCESS` The CVLS initialization was successful.
- `CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CVLS_ILL_INPUT` The CVLS interface is not compatible with the `LS` or `J` input objects or is incompatible with the current NVECTOR module.
- `CVLS_SUNLS_FAIL` A call to the `LS` object failed.
- `CVLS_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 9 for further information).

When using sparse linear solvers, it is typically much more efficient to supply `J` so that it includes the full sparsity pattern of the Newton system matrices $M = I - \gamma J$, even if `J` itself has zeros in nonzero locations of I. The reasoning for this is that M is constructed in-place, on top of the user-specified values of `J`, so if the sparsity pattern in `J` is insufficient to store M then it will need to be resized internally by CVODE.

The previous routines `CVDlsSetLinearSolver` and `CVSpilsSetLinearSolver` 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 `FCVodeSetLinearSolver`

`CVDiag`

Call `flag = CVDiag(cvode_mem);`

Description The function `CVDiag` selects the CVDIAG linear solver.

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

- `CVDIAG_SUCCESS` The CVDIAG initialization was successful.
- `CVDIAG_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CVDIAG_ILL_INPUT` The CVDIAG solver is not compatible with the current NVECTOR module.
- `CVDIAG_MEM_FAIL` A memory allocation request failed.

Notes The CVDIAG solver is the simplest of all of the available CVODES linear solver interfaces. The CVDIAG solver uses an approximate diagonal Jacobian formed by way of a difference quotient. The user does *not* have the option of supplying a function to compute an approximate diagonal Jacobian.

F2003 Name `FCVDiag`

4.5.4 Nonlinear solver interface function

By default CVODES uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §11.3). To specify a different nonlinear solver in CVODES, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object by calling `CVodeSetNonlinearSolver`, as documented below.

When changing the nonlinear solver in CVODES, `CVodeSetNonlinearSolver` must be called after `CVodeInit`. If any calls to `CVode` have been made, then CVODES will need to be reinitialized by calling `CVodeReInit` to ensure that the nonlinear solver is initialized correctly before any subsequent calls to `CVode`.

The first argument passed to the routine `CVodeSetNonlinearSolver` is the CVODES memory pointer returned by `CVodeCreate` and the second argument is the SUNNONLINSOL object to use for solving the nonlinear system (2.4) or (2.5). A call to this function attaches the nonlinear solver to the main CVODES integrator.

`CVodeSetNonlinearSolver`

Call `flag = CVodeSetNonlinearSolver(cvode_mem, NLS);`

Description The function `CVodeSetNonLinearSolver` attaches a SUNNONLINSOL object (`NLS`) to CVODES.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `NLS` (`SUNNonlinearSolver`) SUNNONLINSOL object to use for solving nonlinear systems (2.4) or (2.5).

Return value The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The nonlinear solver was successfully attached.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CV_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 `CV_STAGGERED` or `CV_STAGGERED1` corrector method is used this function sets the nonlinear solver method for correcting state variables (see §5.2.3 for more details).

F2003 Name `FCVodeSetNonlinearSolver`

4.5.5 Rootfinding initialization function

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

`CVodeRootInit`

Call `flag = CVodeRootInit(cvode_mem, nrtfn, g);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `nrtfn` (`int`) is the number of root functions g_i.

	g	(CVRootFn) is the C function which defines the nrtfn functions $g_i(t, y)$ whose roots are sought. See §4.6.4 for details.

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

CV_SUCCESS	The call to CVodeRootInit was successful.
CV_MEM_NULL	The cvode_mem argument was NULL.
CV_MEM_FAIL	A memory allocation failed.
CV_ILL_INPUT	The function g is NULL, but nrtfn > 0.

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

F2003 Name FCVodeRootInit

4.5.6 CVODES solver function

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

CVode

Call `flag = CVode(cvode_mem, tout, yout, &tret, itask);`

Description The function CVode integrates the ODE over an interval in t.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
tout	(realtype) the next time at which a computed solution is desired.
yout	(N_Vector) the computed solution vector.
tret	(realtype) the time reached by the solver (output).
itask	(int) a flag indicating the job of the solver for the next user step. The CV_NORMAL option causes the solver to take internal steps until it has reached or just passed the user-specified tout parameter. The solver then interpolates in order to return an approximate value of y(tout). The CV_ONE_STEP option tells the solver to take just one internal step and then return the solution at the point reached by that step.

Return value CVode returns a vector yout and a corresponding independent variable value $t =$ tret, such that yout is the computed value of $y(t)$.

In CV_NORMAL mode (with no errors), tret will be equal to tout and yout $= y$(tout).

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

CV_SUCCESS	CVode succeeded and no roots were found.
CV_TSTOP_RETURN	CVode succeeded by reaching the stopping point specified through the optional input function CVodeSetStopTime (see §4.5.7.1).
CV_ROOT_RETURN	CVode succeeded and found one or more roots. In this case, tret is the location of the root. If nrtfn > 1, call CVodeGetRootInfo to see which g_i were found to have a root.
CV_MEM_NULL	The cvode_mem argument was NULL.
CV_NO_MALLOC	The CVODES memory was not allocated by a call to CVodeInit.
CV_ILL_INPUT	One of the inputs to CVode 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

	CVodeCreate) failed to set the linear solver-specific lsolve field in cvode_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 error message for details.
CV_TOO_CLOSE	The initial time t_0 and the output time t_{out} are too close to each other and the user did not specify an initial step size.
CV_TOO_MUCH_WORK	The solver took mxstep internal steps but still could not reach tout. The default value for mxstep is MXSTEP_DEFAULT = 500.
CV_TOO_MUCH_ACC	The solver could not satisfy the accuracy demanded by the user for some internal step.
CV_ERR_FAILURE	Either error test failures occurred too many times (MXNEF = 7) during one internal time step, or with $\|h\| = h_{min}$.
CV_CONV_FAILURE	Either convergence test failures occurred too many times (MXNCF = 10) during one internal time step, or with $\|h\| = h_{min}$.
CV_LINIT_FAIL	The linear solver interface's initialization function failed.
CV_LSETUP_FAIL	The linear solver interface's setup function failed in an unrecoverable manner.
CV_LSOLVE_FAIL	The linear solver interface's solve function failed in an unrecoverable manner.
CV_CONSTR_FAIL	The inequality constraints were violated and the solver was unable to recover.
CV_RHSFUNC_FAIL	The right-hand side function failed in an unrecoverable manner.
CV_FIRST_RHSFUNC_FAIL	The right-hand side function had a recoverable error at the first call.
CV_REPTD_RHSFUNC_ERR	Convergence test failures occurred too many times due to repeated recoverable errors in the right-hand side function. This flag will also be returned if the right-hand side function had repeated recoverable errors during the estimation of an initial step size.
CV_UNREC_RHSFUNC_ERR	The right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the right-hand side function fails recoverably after an error test failed while at order one.
CV_RTFUNC_FAIL	The rootfinding function failed.

Notes The vector yout can occupy the same space as the vector y0 of initial conditions that was passed to CVodeInit.

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

If a stop time is enabled (through a call to CVodeSetStopTime), then CVode 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 CVodeSetStopTime).

All failure return values are negative and so the test flag < 0 will trap all CVode failures.

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

F2003 Name FCVode

Table 4.2: Optional inputs for CVODES and CVLS

Optional input	Function name	Default
CVODES main solver		
Pointer to an error file	`CVodeSetErrFile`	`stderr`
Error handler function	`CVodeSetErrHandlerFn`	internal fn.
User data	`CVodeSetUserData`	`NULL`
Maximum order for BDF method	`CVodeSetMaxOrd`	5
Maximum order for Adams method	`CVodeSetMaxOrd`	12
Maximum no. of internal steps before t_{out}	`CVodeSetMaxNumSteps`	500
Maximum no. of warnings for $t_n + h = t_n$	`CVodeSetMaxHnilWarns`	10
Flag to activate stability limit detection	`CVodeSetStabLimDet`	`SUNFALSE`
Initial step size	`CVodeSetInitStep`	estimated
Minimum absolute step size	`CVodeSetMinStep`	0.0
Maximum absolute step size	`CVodeSetMaxStep`	∞
Value of t_{stop}	`CVodeSetStopTime`	undefined
Maximum no. of error test failures	`CVodeSetMaxErrTestFails`	7
Maximum no. of nonlinear iterations	`CVodeSetMaxNonlinIters`	3
Maximum no. of convergence failures	`CVodeSetMaxConvFails`	10
Coefficient in the nonlinear convergence test	`CVodeSetNonlinConvCoef`	0.1
Inequality constraints on solution	`CVodeSetConstraints`	`NULL`
Direction of zero-crossing	`CVodeSetRootDirection`	both
Disable rootfinding warnings	`CVodeSetNoInactiveRootWarn`	none
CVLS linear solver interface		
Jacobian / preconditioner update frequency	`CVodeSetMaxStepsBetweenJac`	50
Jacobian function	`CVodeSetJacFn`	DQ
Linear System function	`CVodeSetLinSysFn`	internal
Jacobian-times-vector functions	`CVodeSetJacTimes`	NULL, DQ
Preconditioner functions	`CVodeSetPreconditioner`	NULL, NULL
Ratio between linear and nonlinear tolerances	`CVodeSetEpsLin`	0.05

4.5.7 Optional input functions

There are numerous optional input parameters that control the behavior of the CVODES solver. CVODES 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 CVODES which are then described in detail in the remainder of this section, begining with those for the main CVODES solver and continuing with those for the linear solver interfaces. Note that the diagonal linear solver module has no optional inputs. For the most casual use of CVODES, the reader can skip to §4.6.

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

4.5.7.1 Main solver optional input functions

The calls listed here can be executed in any order. However, if either of the functions `CVodeSetErrFile` or `CVodeSetErrHandlerFn` is to be called, that call should be first, in order to take effect for any later error message.

`CVodeSetErrFile`

Call `flag = CVodeSetErrFile(cvode_mem, errfp);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`errfp` (`FILE *`) pointer to output file.

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

`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

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

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

If `CVodeSetErrFile` 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 `FCVodeSetErrFile`

`CVodeSetErrHandlerFn`

Call `flag = CVodeSetErrHandlerFn(cvode_mem, ehfun, eh_data);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`ehfun` (`CVErrHandlerFn`) is the 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

`CV_SUCCESS` The function `ehfun` and data pointer `eh_data` have been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

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

F2003 Name `FCVodeSetErrHandlerFn`

`CVodeSetUserData`

Call `flag = CVodeSetUserData(cvode_mem, user_data);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`user_data` (`void *`) pointer to the user data.

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

`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_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 `CVodeSetUserData` must be made *before* the call to specify the linear solver.

F2003 Name `FCVodeSetUserData`

`CVodeSetMaxOrd`

Call `flag = CVodeSetMaxOrd(cvode_mem, maxord);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_ILL_INPUT` The specified value `maxord` is ≤ 0, or larger than its previous value.

Notes The default value is `ADAMS_Q_MAX = 12` for the Adams-Moulton method and `BDF_Q_MAX = 5` for the BDF method. Since `maxord` affects the memory requirements for the internal CVODES memory block, its value cannot be increased past its previous value.

An input value greater than the default will result in the default value.

F2003 Name `FCVodeSetMaxOrd`

`CVodeSetMaxNumSteps`

Call `flag = CVodeSetMaxNumSteps(cvode_mem, mxsteps);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`mxsteps` (`long int`) maximum allowed number of steps.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

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

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

F2003 Name `FCVodeSetMaxNumSteps`

`CVodeSetMaxHnilWarns`

Call `flag = CVodeSetMaxHnilWarns(cvode_mem, mxhnil);`

Description The function `CVodeSetMaxHnilWarns` specifies the maximum number of messages issued by the solver warning that $t + h = t$ on the next internal step.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`mxhnil` (`int`) maximum number of warning messages (> 0).

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The default value is 10. A negative value for `mxhnil` indicates that no warning messages should be issued.

F2003 Name `FCVodeSetMaxHnilWarns`

`CVodeSetStabLimDet`

Call `flag = CVodeSetstabLimDet(cvode_mem, stldet);`

Description The function `CVodeSetStabLimDet` indicates if the BDF stability limit detection algorithm should be used. See §2.3 for further details.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`stldet` (`booleantype`) flag controlling stability limit detection (`SUNTRUE` = on; `SUNFALSE` = off).

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

`CV_SUCCESS` The optional value has been successfully set.

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_ILL_INPUT` The linear multistep method is not set to `CV_BDF`.

Notes The default value is `SUNFALSE`. If `stldet = SUNTRUE` when BDF is used and the method order is greater than or equal to 3, then an internal function, `CVsldet`, is called to detect a possible stability limit. If such a limit is detected, then the order is reduced.

F2003 Name `FCVodeSetStabLimDet`

`CVodeSetInitStep`

Call `flag = CVodeSetInitStep(cvode_mem, hin);`

Description The function `CVodeSetInitStep` specifies the initial step size.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

`CV_SUCCESS` The optional value has been successfully set.

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes By default, CVODES estimates the initial step size to be the solution h of the equation $\|0.5h^2\ddot{y}\|_{\text{WRMS}} = 1$, where $\ddot{y}$ is an estimated second derivative of the solution at `t0`.

F2003 Name `FCVodeSetInitStep`

`CVodeSetMinStep`

Call `flag = CVodeSetMinStep(cvode_mem, hmin);`

Description The function `CVodeSetMinStep` specifies a lower bound on the magnitude of the step size.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`hmin` (`realtype`) minimum absolute value of the step size (≥ 0.0).

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

`CV_SUCCESS` The optional value has been successfully set.

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_ILL_INPUT` Either `hmin` is nonpositive or it exceeds the maximum allowable step size.

Notes The default value is 0.0.

F2003 Name `FCVodeSetMinStep`

`CVodeSetMaxStep`

Call `flag = CVodeSetMaxStep(cvode_mem, hmax);`

Description The function `CVodeSetMaxStep` specifies an upper bound on the magnitude of the step size.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`hmax` (`realtype`) maximum absolute value of the step size (≥ 0.0).

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_ILL_INPUT` Either `hmax` is nonpositive or it is smaller than the minimum allowable step size.

Notes Pass `hmax` $= 0.0$ to obtain the default value ∞.

F2003 Name `FCVodeSetMaxStep`

`CVodeSetStopTime`

Call `flag = CVodeSetStopTime(cvode_mem, tstop);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_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 `CVodeSetStopTime`).

F2003 Name `FCVodeSetStopTime`

`CVodeSetMaxErrTestFails`

Call `flag = CVodeSetMaxErrTestFails(cvode_mem, maxnef);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The default value is 7.

F2003 Name `FCVodeSetMaxErrTestFails`

`CVodeSetMaxNonlinIters`

Call `flag = CVodeSetMaxNonlinIters(cvode_mem, maxcor);`

Description The function `CVodeSetMaxNonlinIters` specifies the maximum number of nonlinear solver iterations permitted per step.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`maxcor` (`int`) maximum number of nonlinear solver iterations allowed per step (> 0).

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

Notes The default value is 3.

F2003 Name `FCVodeSetMaxNonlinIters`

`CVodeSetMaxConvFails`

Call `flag = CVodeSetMaxConvFails(cvode_mem, maxncf);`

Description The function `CVodeSetMaxConvFails` specifies the maximum number of nonlinear solver convergence failures permitted during one step.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`maxncf` (`int`) maximum number of allowable nonlinear solver convergence failures per step (> 0).

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The default value is 10.

F2003 Name `FCVodeSetMaxConvFails`

`CVodeSetNonlinConvCoef`

Call `flag = CVodeSetNonlinConvCoef(cvode_mem, nlscoef);`

Description The function `CVodeSetNonlinConvCoef` specifies the safety factor used in the nonlinear convergence test (see §2.1).

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

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The default value is 0.1.

F2003 Name `FCVodeSetNonlinConvCoef`

`CVodeSetIterType`

Call `flag = CVodeSetIterType(cvode_mem, iter);`

Description The function `CVodeSetIterType` resets the nonlinear solver iteration type to `iter`.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`iter` (`int`) specifies the type of nonlinear solver iteration and may be either `CV_NEWTON` or `CV_FUNCTIONAL`.

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

`CV_SUCCESS`	The optional value has been successfully set.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_ILL_INPUT`	The `iter` value passed is neither `CV_NEWTON` nor `CV_FUNCTIONAL`.

Notes The nonlinear solver iteration type is initially specified in the call to `CVodeCreate` (see §4.5.1). This function call is needed only if `iter` is being changed from its value in the prior call to `CVodeCreate`.

F2003 Name `FCVodeSetIterType`

`CVodeSetConstraints`

Call `flag = CVodeSetConstraints(cvode_mem, constraints);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

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

`CV_SUCCESS`	The optional value has been successfully set.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_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. A `NULL` constraints vector will disable constraint checking.

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 `FCVodeSetConstraints`

4.5.7.2 Linear solver interface optional input functions

The mathematical explanation of the linear solver methods available to CVODES is provided in §2.1. We group the user-callable routines into four categories: general routines concerning the overall CVLS 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.

As discussed in §2.1, CVODES strives to reuse matrix and preconditioner data for as many solves as possible to amortize the high costs of matrix construction and factorization. To that end, CVODES provides a user-callable routine to modify this behavior. To this end, we recall that the Newton system matrices are $M(t,y) = I - \gamma J(t,y)$, where the right-hand side function has Jacobian matrix $J(t,y) = \frac{\partial f(t,y)}{\partial y}$.

The matrix or preconditioner for M can only be updated within a call to the linear solver 'setup' routine. In general, the frequency with which this setup routine is called may be controlled with the `msbj` argument to `CVodeSetMaxStepsBetweenJac`.

`CVodeSetMaxStepsBetweenJac`

Call `retval = CVodeSetMaxStepsBetweenJac(cvode_mem, msbj);`

Description The function `CVodeSetMaxStepsBetweenJac` specifies the maximum number of time steps to wait before recomputation of the Jacobian or recommendation to update the preconditioner.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`msbj` (`long int`) maximum number of time steps to wait before Jacobian/preconditioner reconstruction.

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

`CVLS_SUCCESS` The optional value has been successfully set.

`CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVLS_LMEM_NULL` The CVLS linear solver interface has not been initialized.

Notes If `msbj` is less than 1, the default value of 50 will be used.

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

F2003 Name `FCVodeSetMaxStepsBetweenJac`

When using matrix-based linear solver modules, the CVLS solver interface needs a function to compute an approximation to the Jacobian matrix $J(t, y)$ or the linear system $M = I - \gamma J$. The function to evaluate $J(t, y)$ the must be of type `CVLsJacFn`. 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 CVLS solver. To specify a user-supplied Jacobian function `jac`, CVLS provides the function `CVodeSetJacFn`. The CVLS 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 `CVodeSetUserData`.

`CVodeSetJacFn`

Call `flag = CVodeSetJacFn(cvode_mem, jac);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`jac` (`CVLsJacFn`) user-defined Jacobian approximation function.

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

`CVLS_SUCCESS` The optional value has been successfully set.

`CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVLS_LMEM_NULL` The CVLS linear solver interface has not been initialized.

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

By default, CVLS 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 `CVLsJacFn` is described in §4.6.5.

The previous routine `CVDlsSetJacFn` 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 `FCVodeSetJacFn`

To specify a user-supplied linear system function `linsys`, CVLS provides the function `CVodeSetLinSysFn`. The CVLS interface passes the pointer `user_data` to the linear system function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied linear system function, without using global data in the program. The pointer `user_data` may be specified through `CVodeSetUserData`.

`CVodeSetLinSysFn`

Call `flag = CVodeSetLinSysFn(cvode_mem, linsys);`

Description The function `CVodeSetLinSysFn` specifies the linear system approximation function to be used for a matrix-based solver within the CVLS interface.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`linsys` (`CVLsLinSysFn`) user-defined linear system approximation function.

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

`CVLS_SUCCESS` The optional value has been successfully set.

`CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVLS_LMEM_NULL` The CVLS linear solver interface has not been initialized.

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

By default, CVLS uses an internal linear system function leveraging the SUNMATRIX API to form the system $M = I - \gamma J$ using either an internal finite difference approximation or user-supplied function to compute the Jacobian. If `linsys` is `NULL`, this default function is used.

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

F2003 Name `FCVodeSetLinSysFn`

When using matrix-free linear solver modules, the CVLS 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 CVLS interface. A user-defined Jacobian-vector function must be of type `CVLsJacTimesVecFn` and can be specified through a call to `CVodeSetJacTimes` (see §4.6.7 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 §4.6.8 for specification details).

The pointer `user_data` received through `CVodeSetUserData` (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.

`CVodeSetJacTimes`

Call `flag = CVodeSetJacTimes(cvode_mem, jtsetup, jtimes);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`jtsetup` (`CVLsJacTimesSetupFn`) user-defined Jacobian-vector setup function. Pass `NULL` if no setup is necessary.

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

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

`CVLS_SUCCESS` The optional value has been successfully set.

CVLS_MEM_NULL The cvode_mem pointer is NULL.

CVLS_LMEM_NULL The CVLS linear solver has not been initialized.

CVLS_SUNLS_FAIL An error occurred when setting up the system matrix-times-vector routines in the SUNLINSOL object used by the CVLS 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 CVLS linear solver interface has been initialized through a call to CVodeSetLinearSolver.

The function type CVLsJacTimesSetupFn is described in §4.6.8.

The function type CVLsJacTimesVecFn is described in §4.6.7.

The previous routine CVSpilsSetJacTimes 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 FCVodeSetJacTimes

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 CVODES using the function CVodeSetPreconditioner. 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. The user data pointer received through CVodeSetUserData (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 CVLS interface requires that iterative linear solvers stop when the norm of the preconditioned residual satisfies

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

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

CVodeSetPreconditioner

Call flag = CVodeSetPreconditioner(cvode_mem, psetup, psolve);

Description The function CVodeSetPreconditioner specifies the preconditioner setup and solve functions.

Arguments cvode_mem (void *) pointer to the CVODES memory block.

psetup (CVLsPrecSetupFn) user-defined preconditioner setup function. Pass NULL if no setup is necessary.

psolve (CVLsPrecSolveFn) user-defined preconditioner solve function.

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

CVLS_SUCCESS The optional values have been successfully set.

CVLS_MEM_NULL The cvode_mem pointer is NULL.

CVLS_LMEM_NULL The CVLS linear solver has not been initialized.

CVLS_SUNLS_FAIL An error occurred when setting up preconditioning in the SUNLINSOL object used by the CVLS interface.

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

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

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

The function type `CVLsPrecSetupFn` is described in §4.6.10.

The previous routine `CVSpilsSetPreconditioner` 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 `FCVodeSetPreconditioner`

`CVodeSetEpsLin`

Call `flag = CVodeSetEpsLin(cvode_mem, eplifac);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

`CVLS_SUCCESS` The optional value has been successfully set.

`CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVLS_LMEM_NULL` The CVLS linear solver has not been initialized.

`CVLS_ILL_INPUT` The factor `eplifac` is negative.

Notes The default value is 0.05.

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

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

The previous routine `CVSpilsSetEpsLin` 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 `FCVodeSetEpsLin`

4.5.7.3 Rootfinding optional input functions

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

`CVodeSetRootDirection`

Call `flag = CVodeSetRootDirection(cvode_mem, rootdir);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`rootdir` (`int *`) state array of length `nrtfn`, the number of root functions g_i, as specified in the call to the function `CVodeRootInit`. A value of 0 for `rootdir[i]` indicates that crossing in either direction for g_i should be reported. 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

`CV_SUCCESS` The optional value has been successfully set.

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_ILL_INPUT` rootfinding has not been activated through a call to `CVodeRootInit`.

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

F2003 Name `FCVodeSetRootDirection`

`CVodeSetNoInactiveRootWarn`

Call `flag = CVodeSetNoInactiveRootWarn(cvode_mem);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

`CV_SUCCESS`	The optional value has been successfully set.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.

Notes CVODES 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), CVODES will issue a warning which can be disabled with this optional input function.

F2003 Name `FCVodeSetNoInactiveRootWarn`

4.5.8 Interpolated output function

An optional function `CVodeGetDky` is available to obtain additional output values. This function should only be called after a successful return from `CVode` as it provides interpolated values either of y or of its derivatives (up to the current order of the integration method) interpolated to any value of t in the last internal step taken by CVODES.

The call to the `CVodeGetDky` function has the following form:

`CVodeGetDky`

Call `flag = CVodeGetDky(cvode_mem, t, k, dky);`

Description The function `CVodeGetDky` computes the `k`-th derivative of the function `y` at time `t`, i.e. $d^{(k)}y/dt^{(k)}(t)$, where $t_n - h_u \leq \mathtt{t} \leq t_n$, t_n denotes the current internal time reached, and h_u is the last internal step size successfully used by the solver. The user may request `k` $= 0, 1, \ldots, q_u$, where q_u is the current order (optional output `qlast`).

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`t`	(`realtype`) the value of the independent variable at which the derivative is to be evaluated.
`k`	(`int`) the derivative order requested.
`dky`	(`N_Vector`) vector containing the derivative. This vector must be allocated by the user.

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

`CV_SUCCESS`	`CVodeGetDky` succeeded.
`CV_BAD_K`	`k` is not in the range $0, 1, \ldots, q_u$.
`CV_BAD_T`	`t` is not in the interval $[t_n - h_u, t_n]$.
`CV_BAD_DKY`	The `dky` argument was `NULL`.
`CV_MEM_NULL`	The `cvode_mem` argument was `NULL`.

Notes It is only legal to call the function `CVodeGetDky` after a successful return from `CVode`. See `CVodeGetCurrentTime`, `CVodeGetLastOrder`, and `CVodeGetLastStep` in the next section for access to t_n, q_u, and h_u, respectively.

F2003 Name `FCVodeGetDky`

4.5.9 Optional output functions

CVODES provides an extensive set of functions that can be used to obtain solver performance information. Table 4.3 lists all optional output functions in CVODES, 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 CVODES solver is in doing its job. For example, the counters `nsteps` and `nfevals` 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.

4.5.9.1 SUNDIALS version information

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

`SUNDIALSGetVersion`

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

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

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

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

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

`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.

Table 4.3: Optional outputs from CVODES, CVLS, and CVDIAG

Optional output	Function name
CVODES main solver	
Size of CVODES real and integer workspaces	`CVodeGetWorkSpace`
Cumulative number of internal steps	`CVodeGetNumSteps`
No. of calls to r.h.s. function	`CVodeGetNumRhsEvals`
No. of calls to linear solver setup function	`CVodeGetNumLinSolvSetups`
No. of local error test failures that have occurred	`CVodeGetNumErrTestFails`
Order used during the last step	`CVodeGetLastOrder`
Order to be attempted on the next step	`CVodeGetCurrentOrder`
No. of order reductions due to stability limit detection	`CVodeGetNumStabLimOrderReds`
Actual initial step size used	`CVodeGetActualInitStep`
Step size used for the last step	`CVodeGetLastStep`
Step size to be attempted on the next step	`CVodeGetCurrentStep`
Current internal time reached by the solver	`CVodeGetCurrentTime`
Suggested factor for tolerance scaling	`CVodeGetTolScaleFactor`
Error weight vector for state variables	`CVodeGetErrWeights`
Estimated local error vector	`CVodeGetEstLocalErrors`
No. of nonlinear solver iterations	`CVodeGetNumNonlinSolvIters`
No. of nonlinear convergence failures	`CVodeGetNumNonlinSolvConvFails`
All CVODES integrator statistics	`CVodeGetIntegratorStats`
CVODES nonlinear solver statistics	`CVodeGetNonlinSolvStats`
Array showing roots found	`CVodeGetRootInfo`
No. of calls to user root function	`CVodeGetNumGEvals`
Name of constant associated with a return flag	`CVodeGetReturnFlagName`
CVLS linear solver interface	
Size of real and integer workspaces	`CVodeGetWorkSpace`
No. of Jacobian evaluations	`CVodeGetNumJacEvals`
No. of r.h.s. calls for finite diff. Jacobian[-vector] evals.	`CVodeGetNumLinRhsEvals`
No. of linear iterations	`CVodeGetNumLinIters`
No. of linear convergence failures	`CVodeGetNumLinConvFails`
No. of preconditioner evaluations	`CVodeGetNumPrecEvals`
No. of preconditioner solves	`CVodeGetNumPrecSolves`
No. of Jacobian-vector setup evaluations	`CVodeGetNumJTSetupEvals`
No. of Jacobian-vector product evaluations	`CVodeGetNumJtimesEvals`
Last return from a linear solver function	`CVodeGetLastLinFlag`
Name of constant associated with a return flag	`CVodeGetLinReturnFlagName`
CVDIAG linear solver interface	
Size of CVDIAG real and integer workspaces	`CVDiagGetWorkSpace`
No. of r.h.s. calls for finite diff. Jacobian evals.	`CVDiagGetNumRhsEvals`
Last return from a CVDIAG function	`CVDiagGetLastFlag`
Name of constant associated with a return flag	`CVDiagGetReturnFlagName`

4.5.9.2 Main solver optional output functions

CVODES 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 CVODES memory block (a suggested tolerance scaling factor, the error weight vector, and the vector of estimated local errors). Functions are also provided to extract statistics related to the performance of the CVODES nonlinear solver used. As a convenience, additional information extraction functions provide the optional outputs in groups. These optional output functions are described next.

`CVodeGetWorkSpace`

Call `flag = CVodeGetWorkSpace(cvode_mem, &lenrw, &leniw);`

Description The function `CVodeGetWorkSpace` returns the CVODES real and integer workspace sizes.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`lenrw` (`long int`) the number of `realtype` values in the CVODES workspace.
`leniw` (`long int`) the number of integer values in the CVODES workspace.

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

`CV_SUCCESS` The optional output values have been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

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

- base value: `lenrw` $= 96 +$ (`maxord`+5) $* N_r + 3*$`nrtfn`;
- using `CVodeSVtolerances`: `lenrw` $=$ `lenrw` $+N_r$;
- with constraint checking (see `CVodeSetConstraints`); `lenrw` $=$ `lenrw` $+N_r$;

where 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` $= 40 +$ (`maxord`+5) $* N_i$ $+$ `nrtfn`;
- using `CVodeSVtolerances`: `leniw` $=$ `leniw` $+N_i$;
- with constraint checking: `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 and `npes` processors).

For the default value of `maxord`, no rootfinding, no constraints, and without using `CVodeSVtolerances`, these lengths are given roughly by:

- For the Adams method: `lenrw` $= 96 + 17N$ and `leniw` $= 57$
- For the BDF method: `lenrw` $= 96 + 10N$ and `leniw` $= 50$

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 `FCVodeGetWorkSpace`

`CVodeGetNumSteps`

Call `flag = CVodeGetNumSteps(cvode_mem, &nsteps);`

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

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

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetNumSteps`

`CVodeGetNumRhsEvals`

Call `flag = CVodeGetNumRhsEvals(cvode_mem, &nfevals);`

Description The function `CVodeGetNumRhsEvals` returns the number of calls to the user's right-hand side function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nfevals` (`long int`) number of calls to the user's `f` function.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The `nfevals` value returned by `CVodeGetNumRhsEvals` does not account for calls made to `f` by a linear solver or preconditioner module.

F2003 Name `FCVodeGetNumRhsEvals`

`CVodeGetNumLinSolvSetups`

Call `flag = CVodeGetNumLinSolvSetups(cvode_mem, &nlinsetups);`

Description The function `CVodeGetNumLinSolvSetups` returns the number of calls made to the linear solver's setup function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetNumLinSolvSetups`

`CVodeGetNumErrTestFails`

Call `flag = CVodeGetNumErrTestFails(cvode_mem, &netfails);`

Description The function `CVodeGetNumErrTestFails` returns the number of local error test failures that have occurred.

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

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetNumErrTestFails`

`CVodeGetLastOrder`

Call `flag = CVodeGetLastOrder(cvode_mem, &qlast);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`qlast` (`int`) method order used on the last internal step.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetLastOrder`

`CVodeGetCurrentOrder`

Call `flag = CVodeGetCurrentOrder(cvode_mem, &qcur);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`qcur` (`int`) method order to be used on the next internal step.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetCurrentOrder`

`CVodeGetLastStep`

Call `flag = CVodeGetLastStep(cvode_mem, &hlast);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`hlast` (`realtype`) step size taken on the last internal step.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetLastStep`

`CVodeGetCurrentStep`

Call `flag = CVodeGetCurrentStep(cvode_mem, &hcur);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetCurrentStep`

`CVodeGetActualInitStep`

Call `flag = CVodeGetActualInitStep(cvode_mem, &hinused);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`hinused` (`realtype`) actual value of initial step size.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes Even if the value of the initial integration step size was specified by the user through a call to `CVodeSetInitStep`, this value might have been changed by CVODES to ensure that the step size is within the prescribed bounds ($h_{\min} \le h_0 \le h_{\max}$), or to satisfy the local error test condition.

F2003 Name `FCVodeGetActualInitStep`

`CVodeGetCurrentTime`

Call `flag = CVodeGetCurrentTime(cvode_mem, &tcur);`

Description The function `CVodeGetCurrentTime` returns the current internal time reached by the solver.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`tcur` (`realtype`) current internal time reached.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetCurrentTime`

`CVodeGetNumStabLimOrderReds`

Call `flag = CVodeGetNumStabLimOrderReds(cvode_mem, &nslred);`

Description The function `CVodeGetNumStabLimOrderReds` returns the number of order reductions dictated by the BDF stability limit detection algorithm (see §2.3).

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nslred` (`long int`) number of order reductions due to stability limit detection.

Return value The return value `flag` (of type `int`) is one of
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes If the stability limit detection algorithm was not initialized (`CVodeSetStabLimDet` was not called), then `nslred` = 0.

F2003 Name `FCVodeGetNumStabLimOrderReds`

`CVodeGetTolScaleFactor`

Call `flag = CVodeGetTolScaleFactor(cvode_mem, &tolsfac);`

Description The function `CVodeGetTolScaleFactor` 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 `cvode_mem` (`void *`) pointer to the CVODES memory block.
`tolsfac` (`realtype`) suggested scaling factor for user-supplied tolerances.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetTolScaleFactor`

`CVodeGetErrWeights`

Call `flag = CVodeGetErrWeights(cvode_mem, eweight);`

Description The function `CVodeGetErrWeights` returns the solution error weights at the current time. These are the reciprocals of the W_i given by (2.8).

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`eweight` (`N_Vector`) solution error weights at the current time.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The user must allocate memory for `eweight`.

F2003 Name `FCVodeGetErrWeights`

`CVodeGetEstLocalErrors`

Call `flag = CVodeGetEstLocalErrors(cvode_mem, ele);`

Description The function `CVodeGetEstLocalErrors` returns the vector of estimated local errors.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`ele` (`N_Vector`) estimated local errors.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

Notes The user must allocate memory for `ele`.

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

The `ele` vector, togther with the `eweight` vector from `CVodeGetErrWeights`, 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 `FCVodeGetEstLocalErrors`

`CVodeGetIntegratorStats`

Call
```
flag = CVodeGetIntegratorStats(cvode_mem, &nsteps, &nfevals,
                               &nlinsetups, &netfails, &qlast, &qcur,
                               &hinused, &hlast, &hcur, &tcur);
```

Description The function `CVodeGetIntegratorStats` returns the CVODES integrator statistics as a group.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

nsteps	(long int) number of steps taken by CVODES.
nfevals	(long int) number of calls to the user's f function.
nlinsetups	(long int) number of calls made to the linear solver setup function.
netfails	(long int) number of error test failures.
qlast	(int) method order used on the last internal step.
qcur	(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

CV_SUCCESS	the optional output values have been successfully set.
CV_MEM_NULL	the cvode_mem pointer is NULL.

F2003 Name FCVodeGetIntegratorStats

CVodeGetNumNonlinSolvIters

Call `flag = CVodeGetNumNonlinSolvIters(cvode_mem, &nniters);`

Description The function CVodeGetNumNonlinSolvIters returns the number of nonlinear iterations performed.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
nniters	(long int) number of nonlinear iterations performed.

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

CV_SUCCESS	The optional output values have been successfully set.
CV_MEM_NULL	The cvode_mem pointer is NULL.
CV_MEM_FAIL	The SUNNONLINSOL module is NULL.

F2003 Name FCVodeGetNumNonlinSolvIters

CVodeGetNumNonlinSolvConvFails

Call `flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &nncfails);`

Description The function CVodeGetNumNonlinSolvConvFails returns the number of nonlinear convergence failures that have occurred.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
nncfails	(long int) number of nonlinear convergence failures.

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

CV_SUCCESS	The optional output value has been successfully set.
CV_MEM_NULL	The cvode_mem pointer is NULL.

F2003 Name FCVodeGetNumNonlinSolvConvFails

CVodeGetNonlinSolvStats

Call `flag = CVodeGetNonlinSolvStats(cvode_mem, &nniters, &nncfails);`

Description The function CVodeGetNonlinSolvStats returns the CVODES nonlinear solver statistics as a group.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
nniters	(long int) number of nonlinear iterations performed.

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

F2003 Name `FCVodeGetNonlinSolvStats`

`CVodeGetReturnFlagName`

Call `name = CVodeGetReturnFlagName(flag);`

Description The function `CVodeGetReturnFlagName` returns the name of the CVODES constant corresponding to `flag`.

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

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

F2003 Name `FCVodeGetReturnFlagName`

4.5.9.3 Rootfinding optional output functions

There are two optional output functions associated with rootfinding.

`CVodeGetRootInfo`

Call `flag = CVodeGetRootInfo(cvode_mem, rootsfound);`

Description The function `CVodeGetRootInfo` returns an array showing which functions were found to have a root.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS` The optional output values have been successfully set.

`CV_MEM_NULL` The `cvode_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 `FCVodeGetRootInfo`

`CVodeGetNumGEvals`

Call `flag = CVodeGetNumGEvals(cvode_mem, &ngevals);`

Description The function `CVodeGetNumGEvals` returns the cumulative number of calls made to the user-supplied root function g.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

F2003 Name `FCVodeGetNumGEvals`

4.5.9.4 CVLS linear solver interface optional output functions

The following optional outputs are available from the CVLS modules: workspace requirements, number of calls to the Jacobian routine, number of calls to the right-hand side 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 a linear solver function. Note that, where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix `LS` (for Linear Solver) has been added (e.g. `lenrwLS`).

`CVodeGetLinWorkSpace`

Call `flag = CVodeGetLinWorkSpace(cvode_mem, &lenrwLS, &leniwLS);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `lenrwLS` (`long int`) the number of `realtype` values in the CVLS workspace.
- `leniwLS` (`long int`) the number of integer values in the CVLS workspace.

Return value The return value `flag` (of type `int`) is one of
- `CVLS_SUCCESS` The optional output values have been successfully set.
- `CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CVLS_LMEM_NULL` The CVLS 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 CVLS is not included in this report.

The previous routines `CVDlsGetWorkspace` and `CVSpilsGetWorkspace` 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 `FCVodeGetLinWorkSpace`

`CVodeGetNumJacEvals`

Call `flag = CVodeGetNumJacEvals(cvode_mem, &njevals);`

Description The function `CVodeGetNumJacEvals` returns the number of calls made to the CVLS Jacobian approximation function.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `njevals` (`long int`) the number of calls to the Jacobian function.

Return value The return value `flag` (of type `int`) is one of
- `CVLS_SUCCESS` The optional output value has been successfully set.
- `CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CVLS_LMEM_NULL` The CVLS linear solver has not been initialized.

Notes The previous routine `CVDlsGetNumJacEvals` 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 `FCVodeGetNumJacEvals`

`CVodeGetNumLinRhsEvals`

Call `flag = CVodeGetNumLinRhsEvals(cvode_mem, &nfevalsLS);`

Description The function `CVodeGetNumLinRhsEvals` returns the number of calls made to the user-supplied right-hand side function due to the finite difference Jacobian approximation or finite difference Jacobian-vector product approximation.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nfevalsLS` (`long int`) the number of calls made to the user-supplied right-hand side function.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

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

The previous routines `CVDlsGetNumRhsEvals` and `CVSpilsGetNumRhsEvals` 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 `FCVodeGetNumLinRhsEvals`

`CVodeGetNumLinIters`

Call `flag = CVodeGetNumLinIters(cvode_mem, &nliters);`

Description The function `CVodeGetNumLinIters` returns the cumulative number of linear iterations.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumLinIters` 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 `FCVodeGetNumLinIters`

`CVodeGetNumLinConvFails`

Call `flag = CVodeGetNumLinConvFails(cvode_mem, &nlcfails);`

Description The function `CVodeGetNumLinConvFails` returns the cumulative number of linear convergence failures.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumConvFails` 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 `FCVodeGetNumLinConvFails`

`CVodeGetNumPrecEvals`

Call `flag = CVodeGetNumPrecEvals(cvode_mem, &npevals);`

Description The function `CVodeGetNumPrecEvals` returns the number of preconditioner evaluations, i.e., the number of calls made to `psetup` with `jok = SUNFALSE`.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`npevals` (`long int`) the current number of calls to `psetup`.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumPrecEvals` 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 `FCVodeGetNumPrecEvals`

`CVodeGetNumPrecSolves`

Call `flag = CVodeGetNumPrecSolves(cvode_mem, &npsolves);`

Description The function `CVodeGetNumPrecSolves` returns the cumulative number of calls made to the preconditioner solve function, `psolve`.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`npsolves` (`long int`) the current number of calls to `psolve`.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumPrecSolves` 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 `FCVodeGetNumPrecSolves`

`CVodeGetNumJTSetupEvals`

Call `flag = CVodeGetNumJTSetupEvals(cvode_mem, &njtsetup);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`njtsetup` (`long int`) the current number of calls to `jtsetup`.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumJTSetupEvals` 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 `FCVodeGetNumJTSetupEvals`

`CVodeGetNumJtimesEvals`

Call `flag = CVodeGetNumJtimesEvals(cvode_mem, &njvevals);`

Description The function `CVodeGetNumJtimesEvals` returns the cumulative number of calls made to the Jacobian-vector function `jtimes`.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes The previous routine `CVSpilsGetNumJtimesEvals` 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 `FCVodeGetNumJtimesEvals`

`CVodeGetLastLinFlag`

Call `flag = CVodeGetLastLinFlag(cvode_mem, &lsflag);`

Description The function `CVodeGetLastFlag` returns the last return value from a CVLS routine.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`lsflag` (`long int`) the value of the last return flag from a CVLS function.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.

Notes If the CVLS setup function failed (i.e., `CVode` returned `CV_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 CVLS 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 CVLS solve function failed (i.e., `CVode` returned `CV_LSOLVE_FAIL`), then `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 Jv 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 (SPGMR and SPFGMR only); `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 CVDlsGetLastFlag and CVSpilsGetLastFlag 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 FCVodeGetLastLinFlag

CVodeGetLinReturnFlagName

Call `name = CVodeGetLinReturnFlagName(lsflag);`

Description The function CVodeGetLinReturnFlagName returns the name of the CVLS constant corresponding to lsflag.

Arguments The only argument, of type `long int`, is a return flag from a CVLS 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 routine returns "NONE".

Notes The previous routines CVDlsGetReturnFlagName and CVSpilsGetReturnFlagName 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 FCVodeGetLinReturnFlagName

4.5.9.5 Diagonal linear solver interface optional output functions

The following optional outputs are available from the CVDIAG module: workspace requirements, number of calls to the right-hand side routine for finite-difference Jacobian approximation, and last return value from a CVDIAG function. Note that, where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix LS (for Linear Solver) has been added here (e.g. lenrwLS).

CVDiagGetWorkSpace

Call `flag = CVDiagGetWorkSpace(cvode_mem, &lenrwLS, &leniwLS);`

Description The function CVDiagGetWorkSpace returns the CVDIAG real and integer workspace sizes.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`lenrwLS` (`long int`) the number of `realtype` values in the CVDIAG workspace.
`leniwLS` (`long int`) the number of integer values in the CVDIAG workspace.

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

CVDIAG_SUCCESS	The optional output valus have been successfully set.
CVDIAG_MEM_NULL	The cvode_mem pointer is NULL.
CVDIAG_LMEM_NULL	The CVDIAG linear solver has not been initialized.

Notes In terms of the problem size N, the actual size of the real workspace is roughly $3N$ `realtype` words.

F2003 Name FCVDiagGetWorkSpace

CVDiagGetNumRhsEvals

Call `flag = CVDiagGetNumRhsEvals(cvode_mem, &nfevalsLS);`

Description The function CVDiagGetNumRhsEvals returns the number of calls made to the user-supplied right-hand side function due to the finite difference Jacobian approximation.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nfevalsLS` (`long int`) the number of calls made to the user-supplied right-hand side function.

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

`CVDIAG_SUCCESS`	The optional output value has been successfully set.
`CVDIAG_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVDIAG_LMEM_NULL`	The CVDIAG linear solver has not been initialized.

Notes The number of diagonal approximate Jacobians formed is equal to the number of calls made to the linear solver setup function (see `CVodeGetNumLinSolvSetups`).

F2003 Name `FCVDiagGetNumRhsEvals`

`CVDiagGetLastFlag`

Call `flag = CVDiagGetLastFlag(cvode_mem, &lsflag);`

Description The function `CVDiagGetLastFlag` returns the last return value from a CVDIAG routine.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`lsflag` (`long int`) the value of the last return flag from a CVDIAG function.

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

`CVDIAG_SUCCESS`	The optional output value has been successfully set.
`CVDIAG_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CVDIAG_LMEM_NULL`	The CVDIAG linear solver has not been initialized.

Notes If the CVDIAG setup function failed (`CVode` returned `CV_LSETUP_FAIL`), the value of `lsflag` is equal to `CVDIAG_INV_FAIL`, indicating that a diagonal element with value zero was encountered. The same value is also returned if the CVDIAG solve function failed (`CVode` returned `CV_LSOLVE_FAIL`).

F2003 Name `FCVDiagGetLastFlag`

`CVDiagGetReturnFlagName`

Call `name = CVDiagGetReturnFlagName(lsflag);`

Description The function `CVDiagGetReturnFlagName` returns the name of the CVDIAG constant corresponding to `lsflag`.

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

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

F2003 Name `FCVDiagGetReturnFlagName`

4.5.10 CVODES reinitialization function

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

The use of `CVodeReInit` requires that the maximum method order, denoted by `maxord`, be no larger for the new problem than for the previous problem. This condition is automatically fulfilled if the multistep method parameter `lmm` is unchanged (or changed from `CV_ADAMS` to `CV_BDF`) and the default value for `maxord` is specified.

If there are changes to the linear solver specifications, make the appropriate calls to either the linear solver objects themselves, or to the CVLS interface routines, as described in §4.5.3. Otherwise, all solver inputs set previously remain in effect.

One important use of the `CVodeReInit` function is in the treating of jump discontinuities in the RHS 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 ODE model, using a call to `CVodeReInit`. 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 RHS 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 RHS 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.

`CVodeReInit`

Call `flag = CVodeReInit(cvode_mem, t0, y0);`

Description The function `CVodeReInit` provides required problem specifications and reinitializes CVODES.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `t0` (`realtype`) is the initial value of t.
- `y0` (`N_Vector`) is the initial value of y.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeReInit` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_MALLOC` Memory space for the CVODES memory block was not allocated through a previous call to `CVodeInit`.
- `CV_ILL_INPUT` An input argument to `CVodeReInit` has an illegal value.

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

F2003 Name `FCVodeReInit`

4.6 User-supplied functions

The user-supplied functions consist of one function defining the ODE, (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 iterative algorithms.

4.6.1 ODE right-hand side

The user must provide a function of type `CVRhsFn` defined as follows:

`CVRhsFn`

Definition
```
typedef int (*CVRhsFn)(realtype t, N_Vector y, N_Vector ydot,
                       void *user_data);
```

Purpose This function computes the ODE right-hand side for a given value of the independent variable t and state vector y.

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, $y(t)$.
- `ydot` is the output vector $f(t, y)$.
- `user_data` is the `user_data` pointer passed to `CVodeSetUserData`.

Return value A `CVRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CV_RHSFUNC_FAIL` is returned).

Notes Allocation of memory for `ydot` is handled within CVODES.

A recoverable failure error return from the `CVRhsFn` 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, CVODES 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 right-hand side 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 `CVQuadRhsFn`, which is called at the converged solution of the nonlinear system, and therefore CVODES can be flagged to attempt to recover from such a situation. Also, if sensitivity analysis is performed with one of the staggered methods, the ODE right-hand side function is called at the converged solution of the nonlinear system, and a recoverable error at that point can be flagged, and CVODES will then try to correct it.

There are two other situations in which recovery is not possible even if the right-hand side function returns a recoverable error flag. One is when this occurs at the very first call to the `CVRhsFn` (in which case CVODES returns `CV_FIRST_RHSFUNC_ERR`). The other is when a recoverable error is reported by `CVRhsFn` after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns `CV_UNREC_RHSFUNC_ERR`).

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 `CVodeSetErrFile`), the user may provide a function of type `CVErrHandlerFn` to process any such messages. The function type `CVErrHandlerFn` is defined as follows:

`CVErrHandlerFn`

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

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

Arguments
- `error_code` is the error code.
- `module` is the name of the CVODES 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 `CVodeSetErrHandlerFn`.

Return value A `CVErrHandlerFn` function has no return value.

Notes `error_code` is negative for errors and positive (`CV_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 `CVEwtFn` to compute a vector `ewt` containing the weights in the WRMS norm $\| v\|_{\text{WRMS}} = \sqrt{(1/N)\sum_1^N (W_i \cdot v_i)^2}$. These weights will be used in place of those defined by Eq. (2.8). The function type `CVEwtFn` is defined as follows:

`CVEwtFn`

Definition
```
typedef int (*CVEwtFn)(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 `CVodeSetUserData`.

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

Notes Allocation of memory for `ewt` is handled within CVODES.

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 ODE system, the user must supply a C function of type `CVRootFn`, defined as follows:

`CVRootFn`

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

Purpose This function implements a vector-valued function $g(t, y)$ such that the roots of the `nrtfn` components $g_i(t, y)$ are sought.

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, $y(t)$.
- `gout` is the output array, of length `nrtfn`, with components $g_i(t, y)$.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.

Return value A `CVRootFn` should return 0 if successful or a non-zero value if an error occurred (in which case the integration is halted and `CVode` returns `CV_RTFUNC_FAIL`).

Notes Allocation of memory for `gout` is automatically handled within CVODES.

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 `CVodeSetLinearSolver`), the user may provide a function of type `CVLsJacFn` defined as follows:

`CVLsJacFn`

Definition
```
typedef int (*CVLsJacFn)(realtype t, N_Vector y, N_Vector fy,
                         SUNMatrix Jac, void *user_data,
                         N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the Jacobian matrix $J = \partial f/\partial y$ (or an approximation to it).

Arguments

`t`	is the current value of the independent variable.
`y`	is the current value of the dependent variable vector, namely the predicted value of $y(t)$.
`fy`	is the current value of the vector $f(t, y)$.
`Jac`	is the output Jacobian matrix (of type `SUNMatrix`).
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.
`tmp1`	
`tmp2`	
`tmp3`	are pointers to memory allocated for variables of type `N_Vector` which can be used by a `CVLsJacFn` function as temporary storage or work space.

Return value A `CVLsJacFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct, while CVLS sets `last_flag` to `CVLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `CVodes` returns `CV_LSETUP_FAIL` and CVLS sets `last_flag` to `CVLS_JACFUNC_UNRECVR`).

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 9 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`.

If the user's `CVLsJacFn` function uses difference quotient approximations, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

dense:
A user-supplied dense Jacobian function must load the `N` by `N` dense matrix `Jac` with an approximation to the Jacobian matrix $J(t, y)$ at the point (`t`, `y`). 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 §9.3.

banded:
A user-supplied banded Jacobian function must load the `N` by `N` banded matrix `Jac`

with the elements of the Jacobian $J(t, y)$ at the point (t,y). The accessor macros SM_ELEMENT_B, SM_COLUMN_B, and SM_COLUMN_ELEMENT_B allow the user to read and write band 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 band 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); 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 §9.4.

sparse:
A user-supplied sparse Jacobian function must load the N by N compressed-sparse-column or compressed-sparse-row matrix Jac with an approximation to the Jacobian matrix $J(t, y)$ at the point (t, y). 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 §9.5.

The previous function type CVDlsJacFn is identical to CVLsJacFn, 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 Linear system construction (matrix-based linear solvers)

With matrix-based linear solver modules, as an alternative to optionally supplying a function for evaluating the Jacobian of the ODE right-hand side function, the user may optionally supply a function of type CVLsLinSysFn for evaluating the linear system, $M = I - \gamma J$ (or an approximation of it). CVLsLinSysFn is defined as follows:

CVLsLinSysFn

Definition
```
typedef int (*CVLsLinSysFn)(realtype t, N_Vector y, N_Vector fy,
                            SUNMatrix M, booleantype jok,
                            booleantype *jcur, realtype gamma,
                            void *user_data, N_Vector tmp1,
                            N_Vector tmp2, N_Vector tmp3);
```

Purpose This function computes the linear system matrix $M = I - \gamma J$ (or an approximation to it).

Arguments
- t is the current value of the independent variable.
- y is the current value of the dependent variable vector, namely the predicted value of $y(t)$.

`fy`	is the current value of the vector $f(t, y)$.
`M`	is the output linear system matrix (of type `SUNMatrix`).
`jok`	is an input flag indicating whether the Jacobian-related data needs to be updated. The `jok` flag enables reusing of Jacobian data across linear solves however, the user is responsible for storing Jacobian data for reuse. `jok = SUNFALSE` means that the Jacobian-related data must be recomputed from scratch. `jok = SUNTRUE` means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of `gamma`). A call with `jok = SUNTRUE` can only occur after a call with `jok = SUNFALSE`.
`jcur`	is a pointer to a flag which should be set to `SUNTRUE` if Jacobian data was recomputed, or set to `SUNFALSE` if Jacobian data was not recomputed, but saved data was still reused.
`gamma`	is the scalar γ appearing in the matrix $M = I - \gamma J$.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to the function `CVodeSetUserData`.
`tmp1`	
`tmp2`	
`tmp3`	are pointers to memory allocated for variables of type `N_Vector` which can be used by a `CVLsLinSysFn` function as temporary storage or work space.

Return value A `CVLsLinSysFn` should return `0` if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct, while CVLS sets `last_flag` to `CVLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `CVode` returns `CV_LSETUP_FAIL` and CVLS sets `last_flag` to `CVLS_JACFUNC_UNRECVR`).

4.6.7 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 `CVodeSetLinearSolver`), the user may provide a function of type `CVLsJacTimesVecFn` 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.

`CVLsJacTimesVecFn`

Definition
```
typedef int (*CVLsJacTimesVecFn)(N_Vector v, N_Vector Jv,
                                 realtype t, N_Vector y, N_Vector fy,
                                 void *user_data, N_Vector tmp);
```

Purpose This function computes the product $Jv = (\partial f/\partial y)v$ (or an approximation to it).

Arguments	
`v`	is the vector by which the Jacobian must be multiplied.
`Jv`	is the output vector computed.
`t`	is the current value of the independent variable.
`y`	is the current value of the dependent variable vector.
`fy`	is the current value of the vector $f(t, y)$.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.
`tmp`	is a pointer to memory allocated for a variable of type `N_Vector` which can be used for work space.

Return value The value returned by the Jacobian-vector product function should be 0 if successful. Any other return value will result in an unrecoverable error of the generic Krylov solver, in which case the integration is halted.

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).
If the user's `CVLsJacTimesVecFn` function uses difference quotient approximations, it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `CVSpilsJacTimesVecFn` is identical to `CVLsJacTimesVecFn`, 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 Jacobian-vector product setup (matrix-free linear solvers)

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

`CVLsJacTimesSetupFn`

Definition
```
typedef int (*CVLsJacTimesSetupFn)(realtype t, N_Vector y,
                                   N_Vector fy, void *user_data);
```

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

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector.
- `fy` is the current value of the vector $f(t, y)$.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.

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 `CVRhsFn` user function with the same `(t,y)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.

If the user's `CVLsJacTimesSetupFn` function uses difference quotient approximations, it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `CVSpilsJacTimesSetupFn` is identical to `CVLsJacTimesSetupFn`, 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 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 may be either a left or right preconditioner matrix. Here P should approximate (at least crudely) the matrix $M = I - \gamma J$, where

$J = \partial f/\partial y$. If preconditioning is done on both sides, the product of the two preconditioner matrices should approximate M. This function must be of type `CVLsPrecSolveFn`, defined as follows:

`CVLsPrecSolveFn`

Definition
```
typedef int (*CVLsPrecSolveFn)(realtype t, N_Vector y, N_Vector fy,
                               N_Vector r, N_Vector z, realtype gamma,
                               realtype delta, int lr, void *user_data);
```

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

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector.
- `fy` is the current value of the vector $f(t, y)$.
- `r` is the right-hand side vector of the linear system.
- `z` is the computed output vector.
- `gamma` is the scalar γ appearing in the matrix given by $M = I - \gamma J$.
- `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 the weighted l_2 norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} <$ `delta`. To obtain the `N_Vector ewt`, call `CVodeGetErrWeights` (see §4.5.9.2).
- `lr` is an input flag indicating whether the preconditioner solve function is to use the left preconditioner (`lr = 1`) or the right preconditioner (`lr = 2`);
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to the function `CVodeSetUserData`.

Return value The value 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), or negative for an unrecoverable error (in which case the integration is halted).

Notes The previous function type `CVSpilsPrecSolveFn` is identical to `CVLsPrecSolveFn`, 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.

4.6.10 Preconditioner setup (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 type `CVLsPrecSetupFn`, defined as follows:

`CVLsPrecSetupFn`

Definition
```
typedef int (*CVLsPrecSetupFn)(realtype t, N_Vector y, N_Vector fy,
                               booleantype jok, booleantype *jcurPtr,
                               realtype gamma, void *user_data);
```

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

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, namely the predicted value of $y(t)$.
- `fy` is the current value of the vector $f(t, y)$.
- `jok` is an input flag indicating whether the Jacobian-related data needs to be updated. The `jok` argument provides for the reuse of Jacobian data in the preconditioner solve function. `jok = SUNFALSE` means that the Jacobian-related data must be recomputed from scratch. `jok = SUNTRUE` means that

the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of `gamma`). A call with `jok = SUNTRUE` can only occur after a call with `jok = SUNFALSE`.

`jcurPtr` is a pointer to a flag which should be set to `SUNTRUE` if Jacobian data was recomputed, or set to `SUNFALSE` if Jacobian data was not recomputed, but saved data was still reused.

`gamma` is the scalar γ appearing in the matrix $M = I - \gamma J$.

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

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), or 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 of the resulting approximation to $M = I - \gamma J$.

Each call to the preconditioner setup function is preceded by a call to the `CVRhsFn` user function with the same `(t,y)` arguments. Thus, the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.

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 `CVLsPrecSetupFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.9.2. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `CVSpilsPrecSetupFn` is identical to `CVLsPrecSetupFn`, 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

CVODES allows the ODE 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 vector `y` and excluding the quadrature equations from within `res`. Thus a separate vector `yQ` of quadrature variables is to satisfy $(d/dt)\texttt{yQ} = f_Q(t, y)$. 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.**

   Set the problem size `N` (excluding quadrature variables), and the number of quadrature variables `Nq`.

   If appropriate, set the local vector length `Nlocal` (excluding quadrature variables), and the local number of quadrature variables `Nqlocal`.
3. **Set vector of initial values**
4. **Create CVODES object**

5. **Initialize CVODES 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. **Attach nonlinear solver module**
13. **Set nonlinear solver optional inputs**
14. **Set vector `yQ0` of initial values for quadrature variables**

    Typically, the quadrature variables should be initialized to 0.
15. **Initialize quadrature integration**

    Call `CVodeQuadInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §4.7.1 for details.
16. **Set optional inputs for quadrature integration**

    Call `CVodeSetQuadErrCon` to indicate whether or not quadrature variables shoule be used in the step size control mechanism, and to specify the integration tolerances for quadrature variables. See §4.7.4 for details.
17. **Advance solution in time**
18. **Extract quadrature variables**

    Call `CVodeGetQuad` to obtain the values of the quadrature variables at the current time. See §4.7.3 for details.
19. **Get optional outputs**
20. **Get quadrature optional outputs**

    Call `CVodeGetQuad*` functions to obtain optional output related to the integration of quadratures. See §4.7.5 for details.
21. **Deallocate memory for solution vector and for the vector of quadrature variables**
22. **Free solver memory**
23. **Free nonlinear solver memory**
24. **Free linear solver and matrix memory**
25. **Finalize MPI, if used**

`CVodeQuadInit` can be called and quadrature-related optional inputs (step 16 above) can be set anywhere between steps 4 and 17.

4.7.1 Quadrature initialization and deallocation functions

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

`CVodeQuadInit`

Call `flag = CVodeQuadInit(cvode_mem, fQ, yQ0);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `fQ` (`CVQuadRhsFn`) is the C function which computes f_Q, the right-hand side of the quadrature equations. This function has the form `fQ(t, y, yQdot, fQ_data)` (for full details see §4.7.6).
- `yQ0` (`N_Vector`) is the initial value of `yQ` (typically `yQ0` has all zero components).

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeQuadInit` was successful.
- `CV_MEM_NULL` The CVODES memory was not initialized by a prior call to `CVodeCreate`.
- `CV_MEM_FAIL` A memory allocation request failed.

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

F2003 Name `FCVodeQuadInit`

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 using `CVodeSVtolerances` (see `CVodeSetQuadErrCon`): `lenrw` = `lenrw` +N_q

the size of the integer workspace is increased as follows:

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

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

`CVodeQuadReInit`

Call `flag = CVodeQuadReInit(cvode_mem, yQ0);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `yQ0` (`N_Vector`) is the initial value of `yQ`.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeReInit` was successful.
- `CV_MEM_NULL` The CVODES memory was not initialized by a prior call to `CVodeCreate`.
- `CV_NO_QUAD` Memory space for the quadrature integration was not allocated by a prior call to `CVodeQuadInit`.

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

F2003 Name `FCVodeQuadReInit`

`CVodeQuadFree`

Call `CVodeQuadFree(cvode_mem);`

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

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

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

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

F2003 Name `FCVodeQuadFree`

4.7.2 CVODES solver function

Even if quadrature integration was enabled, the call to the main solver function `CVode` is exactly the same as in §4.5.6. However, in this case the return value `flag` can also be one of the following:

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

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

`CV_REPTD_QRHSFUNC_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).

`CV_UNREC_RHSFUNC_ERR` The quadrature right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the quadrature right-hand side function fails recoverably after an error test failed while at order one.

4.7.3 Quadrature extraction functions

If quadrature integration has been initialized by a call to `CVodeQuadInit`, or reinitialized by a call to `CVodeQuadReInit`, then CVODES computes both a solution and quadratures at time `t`. However, `CVode` will still return only the solution y in `yout`. Solution quadratures can be obtained using the following function:

`CVodeGetQuad`

Call `flag = CVodeGetQuad(cvode_mem, &tret, yQ);`

Description The function `CVodeGetQuad` returns the quadrature solution vector after a successful return from `CVode`.

Arguments
- `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.
- `tret` (`realtype`) the time reached by the solver (output).
- `yQ` (`N_Vector`) the computed quadrature vector. This vector must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuad` is one of:
- `CV_SUCCESS` `CVodeGetQuad` was successful.
- `CV_MEM_NULL` `cvode_mem` was NULL.
- `CV_NO_QUAD` Quadrature integration was not initialized.
- `CV_BAD_DKY` `yQ` is `NULL`.

Notes In case of an error return, an error message is also sent to the error handler function.

F2003 Name `FCVodeGetQuad`

The function CVodeGetQuadDky computes the k-th derivatives of the interpolating polynomials for the quadrature variables at time t. This function is called by CVodeGetQuad with k = 0 and with the current time at which CVode has returned, but may also be called directly by the user.

CVodeGetQuadDky

Call `flag = CVodeGetQuadDky(cvode_mem, t, k, dkyQ);`

Description The function CVodeGetQuadDky returns derivatives of the quadrature solution vector after a successful return from CVode.

Arguments
- `cvode_mem` (`void *`) pointer to the memory previously allocated by CVodeInit.
- `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 CVODES.
- `k` (`int`) order of the requested derivative. This must be $\leq$ qlast.
- `dkyQ` (`N_Vector`) the vector containing the derivative. This vector must be allocated by the user.

Return value The return value flag of CVodeGetQuadDky is one of:
- `CV_SUCCESS` CVodeGetQuadDky succeeded.
- `CV_MEM_NULL` The pointer to cvode_mem was NULL.
- `CV_NO_QUAD` Quadrature integration was not initialized.
- `CV_BAD_DKY` The vector dkyQ is NULL.
- `CV_BAD_K` k is not in the range $0, 1, \ldots,$ qlast.
- `CV_BAD_T` The time t is not in the allowed range.

Notes In case of an error return, an error message is also sent to the error handler function.

F2003 Name `FCVodeGetQuadDky`

4.7.4 Optional inputs for quadrature integration

CVODES provides the following optional input functions to control the integration of quadrature equations.

CVodeSetQuadErrCon

Call `flag = CVodeSetQuadErrCon(cvode_mem, errconQ);`

Description The function CVodeSetQuadErrCon specifies whether or not the quadrature variables are to be used in the step size control mechanism within CVODES. If they are, the user must call CVodeQuadSStolerances or CVodeQuadSVtolerances to specify the integration tolerances for the quadrature variables.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES 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:
- `CV_SUCCESS` The optional value has been successfully set.
- `CV_MEM_NULL` The cvode_mem pointer is NULL.
- `CV_NO_QUAD` Quadrature integration has not been initialized.

Notes By default, errconQ is set to SUNFALSE.

It is illegal to call CVodeSetQuadErrCon before a call to CVodeQuadInit.

F2003 Name `FCVodeSetQuadErrCon`

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.

`CVodeQuadSStolerances`

Call `flag = CVodeQuadSVtolerances(cvode_mem, reltolQ, abstolQ);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional value has been successfully set.
`CV_NO_QUAD`	Quadrature integration was not initialized.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FCVodeQuadSStolerances`

`CVodeQuadSVtolerances`

Call `flag = CVodeQuadSVtolerances(cvode_mem, reltolQ, abstolQ);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional value has been successfully set.
`CV_NO_QUAD`	Quadrature integration was not initialized.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FCVodeQuadSVtolerances`

4.7.5 Optional outputs for quadrature integration

CVODES provides the following functions that can be used to obtain solver performance information related to quadrature integration.

`CVodeGetQuadNumRhsEvals`

Call `flag = CVodeGetQuadNumRhsEvals(cvode_mem, &nfQevals);`

Description The function `CVodeGetQuadNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nfQevals` (`long int`) number of calls made to the user's `fQ` function.

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

`CV_SUCCESS`	The optional output value has been successfully set.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_QUAD`	Quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadNumRhsEvals`

`CVodeGetQuadNumErrTestFails`

Call `flag = CVodeGetQuadNumErrTestFails(cvode_mem, &nQetfails);`

Description The function `CVodeGetQuadNumErrTestFails` returns the number of local error test failures due to quadrature variables.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_QUAD` Quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadNumErrTestFails`

`CVodeGetQuadErrWeights`

Call `flag = CVodeGetQuadErrWeights(cvode_mem, eQweight);`

Description The function `CVodeGetQuadErrWeights` returns the quadrature error weights at the current time.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`eQweight` (`N_Vector`) quadrature error weights at the current time.

Return value The return value `flag` (of type `int`) is one of:
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_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 `CVodeSetQuadErrCon` with `errconQ = SUNTRUE`), `CVodeGetQuadErrWeights` does not set the `eQweight` vector.

F2003 Name `FCVodeGetQuadErrWeights`

`CVodeGetQuadStats`

Call `flag = CVodeGetQuadStats(cvode_mem, &nfQevals, &nQetfails);`

Description The function `CVodeGetQuadStats` returns the CVODES integrator statistics as a group.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nfQevals` (`long int`) number of calls to the user's `fQ` 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
`CV_SUCCESS` the optional output values have been successfully set.
`CV_MEM_NULL` the `cvode_mem` pointer is `NULL`.
`CV_NO_QUAD` Quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadStats`

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 `CVQuadRhsFn` defined as follows:

CVQuadRhsFn

Definition
```
typedef int (*CVQuadRhsFn)(realtype t, N_Vector y,
                           N_Vector yQdot, void *user_data);
```

Purpose This function computes the quadrature equation right-hand side for a given value of the independent variable t and state vector y.

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, $y(t)$.
- `yQdot` is the output vector $f_Q(t, y)$.
- `user_data` is the `user_data` pointer passed to `CVodeSetUserData`.

Return value A `CVQuadRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CV_QRHSFUNC_FAIL` is returned).

Notes Allocation of memory for `yQdot` is automatically handled within CVODES.

Both `y` and `yQdot` 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 CVODES do not perform any consistency checks with respect to their `N_Vector` arguments (see §8.3 and §8.4).

There are two situations in which recovery is not possible even if `CVQuadRhsFn` function returns a recoverable error flag. One is when this occurs at the very first call to the `CVQuadRhsFn` (in which case CVODES returns `CV_FIRST_QRHSFUNC_ERR`). The other is when a recoverable error is reported by `CVQuadRhsFn` after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns `CV_UNREC_QRHSFUNC_ERR`).

4.8 Preconditioner modules

The efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. For problems in which the user cannot define a more effective, problem-specific preconditioner, CVODES provides a banded preconditioner in the module CVBANDPRE and a band-block-diagonal preconditioner module CVBBDPRE.

4.8.1 A serial banded preconditioner module

This preconditioner provides a band matrix preconditioner for use with iterative SUNLINSOL modules through the CVLS linear solver interface, in a serial setting. It uses difference quotients of the ODE right-hand side function `f` to generate a band matrix of bandwidth $m_l + m_u + 1$, where the number of super-diagonals (m_u, the upper half-bandwidth) and sub-diagonals (m_l, the lower half-bandwidth) are specified by the user, and uses this to form a preconditioner for use with the Krylov linear solver. Although this matrix is intended to approximate the Jacobian $\partial f/\partial y$, it may be a very crude approximation. The true Jacobian need not be banded, or its true bandwidth may be larger than $m_l + m_u + 1$, as long as the banded approximation generated here is sufficiently accurate to speed convergence as a preconditioner.

In order to use the CVBANDPRE module, the user need not define any additional functions. Aside from the header files required for the integration of the ODE problem (see §4.3), to use the CVBANDPRE module, the main program must include the header file `cvodes_bandpre.h` which declares the needed function prototypes. The following is a summary of the usage of this module. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. **Initialize multi-threaded environment, if appropriate**
2. **Set problem dimensions etc.**
3. **Set vector of initial values**
4. **Create CVODES object**
5. **Initialize CVODES solver**
6. **Specify integration tolerances**
7. **Create linear solver object**

   When creating the iterative linear solver object, specify the type of preconditioning (`PREC_LEFT` or `PREC_RIGHT`) to use.
8. **Set linear solver optional inputs**
9. **Attach linear solver module**
10. **Initialize the CVBANDPRE preconditioner module**

    Specify the upper and lower half-bandwidths (`mu` and `ml`, respectively) and call

    ```
    flag = CVBandPrecInit(cvode_mem, N, mu, ml);
    ```

    to allocate memory and initialize the internal preconditioner data.
11. **Set optional inputs**

    Note that the user should not overwrite the preconditioner setup function or solve function through calls to the `CVodeSetPreconditioner` optional input function.
12. **Create nonlinear solver object**
13. **Attach nonlinear solver module**
14. **Set nonlinear solver optional inputs**
15. **Specify rootfinding problem**
16. **Advance solution in time**
17. **Get optional outputs**

    Additional optional outputs associated with CVBANDPRE are available by way of two routines described below, `CVBandPrecGetWorkSpace` and `CVBandPrecGetNumRhsEvals`.
18. **Deallocate memory for solution vector**
19. **Free solver memory**
20. **Free nonlinear solver memory**
21. **Free linear solver memory**

The CVBANDPRE preconditioner module is initialized and attached by calling the following function:

`CVBandPrecInit`

Call `flag = CVBandPrecInit(cvode_mem, N, mu, ml);`

Description The function `CVBandPrecInit` initializes the CVBANDPRE preconditioner and allocates required (internal) memory for it.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`N` (`sunindextype`) problem dimension.
`mu` (`sunindextype`) upper half-bandwidth of the Jacobian approximation.
`ml` (`sunindextype`) lower half-bandwidth of the Jacobian approximation.

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

`CVLS_SUCCESS` The call to `CVBandPrecInit` was successful.
`CVLS_MEM_NULL` The `cvode_mem` pointer was `NULL`.
`CVLS_MEM_FAIL` A memory allocation request has failed.
`CVLS_LMEM_NULL` A CVLS linear solver memory was not attached.
`CVLS_ILL_INPUT` The supplied vector implementation was not compatible with block band preconditioner.

Notes The banded approximate Jacobian will have nonzero elements only in locations (i, j) with $-\texttt{ml} \leq j - i \leq \texttt{mu}$.

F2003 Name `FCVBandPrecInit`

The following three optional output functions are available for use with the CVBANDPRE module:

`CVBandPrecGetWorkSpace`

Call `flag = CVBandPrecGetWorkSpace(cvode_mem, &lenrwBP, &leniwBP);`

Description The function `CVBandPrecGetWorkSpace` returns the sizes of the CVBANDPRE real and integer workspaces.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`lenrwBP` (`long int`) the number of `realtype` values in the CVBANDPRE workspace.
`leniwBP` (`long int`) the number of integer values in the CVBANDPRE workspace.

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

`CVLS_SUCCESS` The optional output values have been successfully set.
`CVLS_PMEM_NULL` The CVBANDPRE preconditioner has not been initialized.

Notes The workspace requirements reported by this routine correspond only to memory allocated within the CVBANDPRE module (the banded matrix approximation, banded SUNLINSOL object, and temporary vectors).

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

F2003 Name `FCVBandPrecGetWorkSpace`

`CVBandPrecGetNumRhsEvals`

Call `flag = CVBandPrecGetNumRhsEvals(cvode_mem, &nfevalsBP);`

Description The function `CVBandPrecGetNumRhsEvals` returns the number of calls made to the user-supplied right-hand side function for the finite difference banded Jacobian approximation used within the preconditioner setup function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nfevalsBP` (`long int`) the number of calls to the user right-hand side function.

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

`CVLS_SUCCESS` The optional output value has been successfully set.
`CVLS_PMEM_NULL` The CVBANDPRE preconditioner has not been initialized.

Notes The counter `nfevalsBP` is distinct from the counter `nfevalsLS` returned by the corresponding function `CVodeGetNumLinRhsEvals` and `nfevals` returned by `CVodeGetNumRhsEvals`. The total number of right-hand side function evaluations is the sum of all three of these counters.

F2003 Name `FCVBandPrecGetNumRhsEvals`

4.8.2 A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel ODE solver such as CVODES 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 (2.6) 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 [34] and is included in a software module within the CVODES package. This module works with the parallel vector module NVECTOR_PARALLEL and is usable with any of the Krylov iterative linear solvers through the CVLS interface. It 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 CVBBDPRE.

One way to envision these preconditioners is to think of the domain of the computational PDE problem as being subdivided into M non-overlapping subdomains. Each of these subdomains is then assigned to one of the M processes to be used to solve the ODE system. The basic idea is to isolate the preconditioning so that it is local to each process, and also to use a (possibly cheaper) approximate right-hand side function. This requires the definition of a new function $g(t, y)$ which approximates the function $f(t, y)$ in the definition of the ODE system (2.1). However, the user may set $g = f$. Corresponding to the domain decomposition, there is a decomposition of the solution vector y into M disjoint blocks y_m, and a decomposition of g into blocks g_m. The block g_m depends both on y_m and on components of blocks $y_{m'}$ associated with neighboring subdomains (so-called ghost-cell data). Let $\bar{y}_m$ denote y_m augmented with those other components on which g_m depends. Then we have

$$g(t, y) = [g_1(t, \bar{y}_1), g_2(t, \bar{y}_2), \ldots, g_M(t, \bar{y}_M)]^T \tag{4.1}$$

and each of the blocks $g_m(t, \bar{y}_m)$ is uncoupled from the others.

The preconditioner associated with this decomposition has the form

$$P = \mathrm{diag}[P_1, P_2, \ldots, P_M] \tag{4.2}$$

where

$$P_m \approx I - \gamma J_m \tag{4.3}$$

and J_m is a difference quotient approximation to $\partial g_m / \partial y_m$. 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 Jacobian of the local block of g, if smaller values provide a more efficient preconditioner. The solution of the complete linear system

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

reduces to solving each of the equations

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

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

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

The CVBBDPRE module calls two user-provided functions to construct P: a required function `gloc` (of type `CVLocalFn`) which approximates the right-hand side function $g(t, y) \approx f(t, y)$ and which is computed locally, and an optional function `cfn` (of type `CVCommFn`) which performs all interprocess communication necessary to evaluate the approximate right-hand side g. These are in addition to the user-supplied right-hand side function `f`. Both functions take as input the same pointer `user_data` that is passed by the user to `CVodeSetUserData` and that was passed to the user's function `f`. The user is responsible for providing space (presumably within `user_data`) for components of `y` that are communicated between processes by `cfn`, and that are then used by `gloc`, which should not do any communication.

`CVLocalFn`

Definition
```
typedef int (*CVLocalFn)(sunindextype Nlocal, realtype t, N_Vector y,
                         N_Vector glocal, void *user_data);
```

Purpose This `gloc` function computes $g(t, y)$. It loads the vector `glocal` as a function of `t` and `y`.

Arguments
- `Nlocal` is the local vector length.
- `t` is the value of the independent variable.
- `y` is the dependent variable.
- `glocal` is the output vector.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.

Return value A `CVLocalFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVode` returns `CV_LSETUP_FAIL`).

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

The case where g is mathematically identical to f is allowed.

`CVCommFn`

Definition
```
typedef int (*CVCommFn)(sunindextype Nlocal, realtype t,
                        N_Vector y, void *user_data);
```

Purpose This `cfn` function performs all interprocess communication necessary for the execution of the `gloc` function above, using the input vector `y`.

Arguments
- `Nlocal` is the local vector length.
- `t` is the value of the independent variable.
- `y` is the dependent variable.
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.

Return value A `CVCommFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVode` returns `CV_LSETUP_FAIL`).

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

Each call to the `cfn` function is preceded by a call to the right-hand side function `f` with the same (`t`, `y`) arguments. Thus, `cfn` can omit any communication done by `f`

if relevant to the evaluation of `glocal`. If all necessary communication was done in `f`, then `cfn = NULL` can be passed in the call to `CVBBDPrecInit` (see below).

Besides the header files required for the integration of the ODE problem (see §4.3), to use the CVBBDPRE module, the main program must include the header file `cvodes_bbdpre.h` which declares the needed function prototypes.

The following is a summary of the proper usage of this module. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. **Initialize MPI environment**
2. **Set problem dimensions etc.**
3. **Set vector of initial values**
4. **Create CVODES object**
5. **Initialize CVODES solver**
6. **Specify integration tolerances**
7. **Create linear solver object**

   When creating the iterative linear solver object, specify the type of preconditioning (`PREC_LEFT` or `PREC_RIGHT`) to use.
8. **Set linear solver optional inputs**
9. **Attach linear solver module**
10. **Initialize the CVBBDPRE preconditioner module**

    Specify the upper and lower half-bandwidths `mudq` and `mldq`, and `mukeep` and `mlkeep`, and call

    ```
    flag = CVBBDPrecInit(cvode_mem, local_N, mudq, mldq,
                         mukeep, mlkeep, dqrely, gloc, cfn);
    ```

    to allocate memory and initialize the internal preconditioner data. The last two arguments of `CVBBDPrecInit` are the two user-supplied functions described above.
11. **Set optional inputs**

    Note that the user should not overwrite the preconditioner setup function or solve function through calls to the `CVodeSetPreconditioner` optional input function.
12. **Create nonlinear solver object**
13. **Attach nonlinear solver module**
14. **Set nonlinear solver optional inputs**
15. **Specify rootfinding problem**
16. **Advance solution in time**
17. **Get optional outputs**

    Additional optional outputs associated with CVBBDPRE are available by way of two routines described below, `CVBBDPrecGetWorkSpace` and `CVBBDPrecGetNumGfnEvals`.
18. **Deallocate memory for solution vector**
19. **Free solver memory**

20. **Free nonlinear solver memory**

21. **Free linear solver memory**

22. **Finalize MPI**

The user-callable functions that initialize (step 10 above) or re-initialize the CVBBDPRE preconditioner module are described next.

`CVBBDPrecInit`

Call
```
flag = CVBBDPrecInit(cvode_mem, local_N, mudq, mldq,
                     mukeep, mlkeep, dqrely, gloc, cfn);
```

Description The function `CVBBDPrecInit` initializes and allocates (internal) memory for the CVBBDPRE preconditioner.

Arguments

`cvode_mem`	(`void *`) pointer to the CVODES memory block.
`local_N`	(`sunindextype`) local vector length.
`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.
`dqrely`	(`realtype`) the relative increment in components of `y` used in the difference quotient approximations. The default is `dqrely`$= \sqrt{\text{unit roundoff}}$, which can be specified by passing `dqrely` $= 0.0$.
`gloc`	(`CVLocalFn`) the C function which computes the approximation $g(t, y) \approx f(t, y)$.
`cfn`	(`CVCommFn`) the optional C function which performs all interprocess communication required for the computation of $g(t, y)$.

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

`CVLS_SUCCESS`	The call to `CVBBDPrecInit` was successful.
`CVLS_MEM_NULL`	The `cvode_mem` pointer was `NULL`.
`CVLS_MEM_FAIL`	A memory allocation request has failed.
`CVLS_LMEM_NULL`	A CVLS linear solver was not attached.
`CVLS_ILL_INPUT`	The supplied vector implementation was not compatible with block band preconditioner.

Notes If one of the half-bandwidths `mudq` or `mldq` to be used in the difference quotient calculation of the approximate Jacobian is negative or exceeds the value `local_N`-1, it is replaced by 0 or `local_N`-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 computational costs further.

For all four half-bandwidths, the values need not be the same on every processor.

F2003 Name `FCVBBDPrecInit`

The CVBBDPRE module also provides a reinitialization function to allow solving 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 `CVodeReInit` to re-initialize CVODES for a subsequent problem, a call to `CVBBDPrecReInit` 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 `dqrely`, or one of the user-supplied functions `gloc` and `cfn`. 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 CVLS "set" functions, must also be made (in the proper order).

`CVBBDPrecReInit`

Call `flag = CVBBDPrecReInit(cvode_mem, mudq, mldq, dqrely);`

Description The function `CVBBDPrecReInit` re-initializes the CVBBDPRE preconditioner.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES 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.
- `dqrely` (`realtype`) the relative increment in components of `y` used in the difference quotient approximations. The default is `dqrely` $= \sqrt{\text{unit roundoff}}$, which can be specified by passing `dqrely` $= 0.0$.

Return value The return value `flag` (of type `int`) is one of
- `CVLS_SUCCESS` The call to `CVBBDPrecReInit` was successful.
- `CVLS_MEM_NULL` The `cvode_mem` pointer was `NULL`.
- `CVLS_LMEM_NULL` A CVLS linear solver memory was not attached.
- `CVLS_PMEM_NULL` The function `CVBBDPrecInit` was not previously called.

Notes If one of the half-bandwidths `mudq` or `mldq` is negative or exceeds the value `local_N`-1, it is replaced by 0 or `local_N`-1 accordingly.

F2003 Name `FCVBBDPrecReInit`

The following two optional output functions are available for use with the CVBBDPRE module:

`CVBBDPrecGetWorkSpace`

Call `flag = CVBBDPrecGetWorkSpace(cvode_mem, &lenrwBBDP, &leniwBBDP);`

Description The function `CVBBDPrecGetWorkSpace` returns the local CVBBDPRE real and integer workspace sizes.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `lenrwBBDP` (`long int`) local number of `realtype` values in the CVBBDPRE workspace.
- `leniwBBDP` (`long int`) local number of integer values in the CVBBDPRE workspace.

Return value The return value `flag` (of type `int`) is one of
- `CVLS_SUCCESS` The optional output value has been successfully set.
- `CVLS_MEM_NULL` The `cvode_mem` pointer was `NULL`.
- `CVLS_PMEM_NULL` The CVBBDPRE preconditioner has not been initialized.

Notes The workspace requirements reported by this routine correspond only to memory allocated within the CVBBDPRE 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 `CVodeGetLinWorkSpace`.

F2003 Name `FCVBBDPrecGetWorkSpace`

`CVBBDPrecGetNumGfnEvals`

Call `flag = CVBBDPrecGetNumGfnEvals(cvode_mem, &ngevalsBBDP);`

Description The function `CVBBDPrecGetNumGfnEvals` returns the number of calls made to the user-supplied `gloc` function due to the finite difference approximation of the Jacobian blocks used within the preconditioner setup function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`ngevalsBBDP` (`long int`) the number of calls made to the user-supplied `gloc` function.

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

`CVLS_SUCCESS`	The optional output value has been successfully set.
`CVLS_MEM_NULL`	The `cvode_mem` pointer was `NULL`.
`CVLS_PMEM_NULL`	The CVBBDPRE preconditioner has not been initialized.

F2003 Name `FCVBBDPrecGetNumGfnEvals`

In addition to the `ngevalsBBDP` `gloc` evaluations, the costs associated with CVBBDPRE also include `nlinsetups` LU factorizations, `nlinsetups` calls to `cfn`, `npsolves` banded backsolve calls, and `nfevalsLS` right-hand side function evaluations, where `nlinsetups` is an optional CVODES output and `npsolves` and `nfevalsLS` are linear solver optional outputs (see §4.5.9).

Chapter 5

Using CVODES for Forward Sensitivity Analysis

This chapter describes the use of CVODES to compute solution sensitivities using forward sensitivity analysis. One of our main guiding principles was to design the CVODES 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 right-hand side of the sensitivity systems (2.12). The only departure from this philosophy is due to the `CVRhsFn` type definition (§4.6.1). Without changing the definition of this type, the only way to pass values of the problem parameters to the ODE right-hand side function is to require the user data structure `f_data` to contain a pointer to the array of real parameters p.

CVODES 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 CVODES. 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 8, 9, 10, and 11 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 vector of initial values**
4. **Create CVODES object**
5. **Initialize CVODES 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 CVODES is to evaluate the right-hand sides 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 right-hand side, `p` need not be specified.

    •Parameter list (optional)

    If CVODES is to evaluate the right-hand sides of the sensitivity systems, 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]` are desired ($0 \le$ `j` $<$ `Np`), set $\text{plist}_i = j$, for some $i = 0, \ldots, N_s - 1$.

    If `plist` is not specified, CVODES 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 right-hand side, `plist` need not be specified.

    •Parameter scaling factors (optional)

    If CVODES is to estimate tolerances for the sensitivity solution vectors (based on tolerances for the state solution vector) or if CVODES is to evaluate the right-hand sides 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, CVODES will use $\bar{p}_i = 1.0$.

    If the user provides a function to evaluate the sensitivity right-hand side 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 `CVodeSetSensParams` below.

17. **Set sensitivity initial conditions**

    Set the `Ns` vectors `yS0[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]`.

18. **Activate sensitivity calculations**

    Call `flag = CVodeSensInit` or `CVodeSensInit1` to activate forward sensitivity computations and allocate internal memory for CVODES related to sensitivity calculations (see §5.2.1).

19. **Set sensitivity tolerances**

    Call `CVodeSensSStolerances`, `CVodeSensSVtolerances` or `CVodeEEtolerances`. (See §5.2.2).

20. **Set sensitivity analysis optional inputs**

    Call `CVodeSetSens*` routines to change from their default values any optional inputs that control the behavior of CVODES in computing forward sensitivities. (See §5.2.6.)

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(...);
    ```

    for the `CV_SIMULTANEOUS` or `CV_STAGGERED` options or

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

    for the `CV_STAGGERED1` option where `***` is the name of the nonlinear solver and `...` are constructor specific arguments (see Chapter 11 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 = CVodeSetNonlinearSolverSensSim(cvode_mem, NLSSens);
    ```

    when using the `CV_SIMULTANEOUS` corrector method,

    ```
    ier = CVodeSetNonlinearSolverSensStg(cvode_mem, NLSSens);
    ```

    when using the `CV_STAGGERED` corrector method, or

    ```
    ier = CVodeSetNonlinearSolverSensStg1(cvode_mem, NLSSens);
    ```

    when using the `CV_STAGGERED1` 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 `CVodeSensInit` if using the default nonlinear solver or after attaching a new nonlinear solver to CVODES, otherwise the optional inputs will be overridden by CVODE defaults. See Chapter 11 for more information on optional inputs.

24. **Specify rootfinding**

25. **Advance solution in time**

26. **Extract sensitivity solution**

    After each successful return from `CVode`, the solution of the original IVP is available in the `y` argument of `CVode`, while the sensitivity solution can be extracted into `yS` (which can be the same as `yS0`) by calling one of the routines `CVodeGetSens`,`CVodeGetSens1`, `CVodeGetSensDky`, or `CVodeGetSensDky1` (see §5.2.5).

27. **Get optional outputs**

28. **Deallocate memory for solution vector**

29. **Deallocate memory for sensitivity vectors**

    Upon completion of the integration, deallocate memory for the vectors `yS0` using the appropriate destructor:

    ```
    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 `yS0_i`.

30. **Free user data structure**

31. **Free solver memory**

32. **Free nonlinear solver memory**

33. **Free vector specification memory**

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

35. **Finalize MPI, if used**

5.2 User-callable routines for forward sensitivity analysis

This section describes the CVODES functions, in addition to those presented in §4.5, that are called by the user to setup and solve a forward sensitivity problem.

5.2.1 Forward sensitivity initialization and deallocation functions

Activation of forward sensitivity computation is done by calling `CVodeSensInit` or `CVodeSensInit1`, depending on whether the sensitivity right-hand side function returns all sensitivities at once or one by one, respectively. The form of the call to each of these routines is as follows:

`CVodeSensInit`

Call `flag = CVodeSensInit(cvode_mem, Ns, ism, fS, yS0);`

Description The routine `CVodeSensInit` activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `Ns` (`int`) the number of sensitivities to be computed.
- `ism` (`int`) a flag used to select the sensitivity solution method. Its value can be `CV_SIMULTANEOUS` or `CV_STAGGERED`:
  - In the `CV_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 `CV_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;
- `fS` (`CVSensRhsFn`) is the C function which computes all sensitivity ODE right-hand sides at the same time. For full details see §5.3.
- `yS0` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeSensInit` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_MEM_FAIL` A memory allocation request has failed.
- `CV_ILL_INPUT` An input argument to `CVodeSensInit` has an illegal value.

Notes Passing `fS=NULL` indicates using the default internal difference quotient sensitivity right-hand side routine.

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

It is illegal here to use `ism` = `CV_STAGGERED1`. This option requires a different type for `fS` and can therefore only be used with `CVodeSensInit1` (see below).

F2003 Name `FCVodeSensInit`

`CVodeSensInit1`

Call `flag = CVodeSensInit1(cvode_mem, Ns, ism, fS1, yS0);`

Description The routine `CVodeSensInit1` activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `Ns` (`int`) the number of sensitivities to be computed.
- `ism` (`int`) a flag used to select the sensitivity solution method. Its value can be `CV_SIMULTANEOUS`, `CV_STAGGERED`, or `CV_STAGGERED1`:
  - In the `CV_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 `CV_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;

- In the CV_STAGGERED1 approach, all corrections are done sequentially, first for the state variables and then for the sensitivity variables, one parameter at a time. If the sensitivity variables are not included in the error control, this approach is equivalent to CV_STAGGERED. Note that the CV_STAGGERED1 approach can be used only if the user-provided sensitivity right-hand side function is of type CVSensRhs1Fn (see §5.3).

fS1 (CVSensRhs1Fn) is the C function which computes the right-hand sides of the sensitivity ODE, one at a time. For full details see §5.3.

yS0 (N_Vector *) a pointer to an array of Ns vectors containing the initial values of the sensitivities.

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

CV_SUCCESS The call to CVodeSensInit1 was successful.

CV_MEM_NULL The CVODES memory block was not initialized through a previous call to CVodeCreate.

CV_MEM_FAIL A memory allocation request has failed.

CV_ILL_INPUT An input argument to CVodeSensInit1 has an illegal value.

Notes Passing fS1=NULL indicates using the default internal difference quotient sensitivity right-hand side routine.

If an error occurred, CVodeSensInit1 also sends an error message to the error handler funciton.

F2003 Name FCVodeSensInit1

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 CVodeSensSVtolerances: 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 CVodeSensSVtolerances: leniw = leniw +$N_s N_i$

where N_i is the number of integers in one N_Vector.

The routine CVodeSensReInit, useful during the solution of a sequence of problems of same size, reinitializes the sensitivity-related internal memory. The call to it must follow a call to CVodeSensInit or CVodeSensInit1 (and maybe a call to CVodeReInit). The number Ns of sensitivities is assumed to be unchanged since the call to the initialization function. The call to the CVodeSensReInit function has the form:

CVodeSensReInit

Call flag = CVodeSensReInit(cvode_mem, ism, yS0);

Description The routine CVodeSensReInit reinitializes forward sensitivity computations.

Arguments cvode_mem (void *) pointer to the CVODES memory block returned by CVodeCreate.

ism (int) a flag used to select the sensitivity solution method. Its value can be CV_SIMULTANEOUS, CV_STAGGERED, or CV_STAGGERED1.

yS0 (N_Vector *) a pointer to an array of Ns variables of type N_Vector containing the initial values of the sensitivities.

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

CV_SUCCESS The call to CVodeReInit was successful.

CV_MEM_NULL	The CVODES memory block was not initialized through a previous call to CVodeCreate.
CV_NO_SENS	Memory space for sensitivity integration was not allocated through a previous call to CVodeSensInit.
CV_ILL_INPUT	An input argument to CVodeSensReInit has an illegal value.
CV_MEM_FAIL	A memory allocation request has failed.

Notes All arguments of CVodeSensReInit are the same as those of the functions CVodeSensInit and CVodeSensInit1.

If an error occurred, CVodeSensReInit also sends a message to the error handler function.

CVodeSensReInit potentially does some minimal memory allocation (for the sensitivity absolute tolerance) and for arrays of counters used by the CV_STAGGERED1 method.

The value of the input argument ism must be compatible with the type of the sensitivity ODE right-hand side function. Thus if the sensitivity module was initialized using CVodeSensInit, then it is illegal to pass ism = CV_STAGGERED1 to CVodeSensReInit.

F2003 Name FCVodeSensReInit

To deallocate all forward sensitivity-related memory (allocated in a prior call to CVodeSensInit or CVodeSensInit1), the user must call

CVodeSensFree

Call CVodeSensFree(cvode_mem);

Description The function CVodeSensFree frees the memory allocated for forward sensitivity computations by a previous call to CVodeSensInit or CVodeSensInit1.

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

Return value The function CVodeSensFree has no return value.

Notes In general, CVodeSensFree need not be called by the user, as it is invoked automatically by CVodeFree.

After a call to CVodeSensFree, forward sensitivity computations can be reactivated only by calling CVodeSensInit or CVodeSensInit1 again.

F2003 Name FCVodeSensFree

To activate and deactivate forward sensitivity calculations for successive CVODES runs, without having to allocate and deallocate memory, the following function is provided:

CVodeSensToggleOff

Call CVodeSensToggleOff(cvode_mem);

Description The function CVodeSensToggleOff deactivates forward sensitivity calculations. It does *not* deallocate sensitivity-related memory.

Arguments cvode_mem (void *) pointer to the memory previously returned by CVodeCreate.

Return value The return value flag of CVodeSensToggle is one of:

CV_SUCCESS CVodeSensToggleOff was successful.

CV_MEM_NULL cvode_mem was NULL.

Notes Since sensitivity-related memory is not deallocated, sensitivities can be reactivated at a later time (using CVodeSensReInit).

F2003 Name FCVodeSensToggleOff

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 `CVodeSensInit`/`CVodeSensInit1`.

`CVodeSensSStolerances`

Call `flag = CVodeSensSStolerances(cvode_mem, reltolS, abstolS);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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, one for each parameter.

Return value The return flag `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeSStolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_SENS` The sensitivity allocation function (`CVodeSensInit` or `CVodeSensInit1`) has not been called.
- `CV_ILL_INPUT` One of the input tolerances was negative.

F2003 Name `FCVodeSensSStolerances`

`CVodeSensSVtolerances`

Call `flag = CVodeSensSVtolerances(cvode_mem, reltolS, abstolS);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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:
- `CV_SUCCESS` The call to `CVodeSVtolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_SENS` The allocation function for sensitivities has not been called.
- `CV_ILL_INPUT` The relative error tolerance was negative or an absolute tolerance vector 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 `FCVodeSensSVtolerances`

`CVodeSensEEtolerances`

Call `flag = CVodeSensEEtolerances(cvode_mem);`

Description When `CVodeSensEEtolerances` is called, CVODES will estimate tolerances for sensitivity variables based on the tolerances supplied for states variables and the scaling factors $\bar{p}$.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.

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

CV_SUCCESS	The call to CVodeSensEEtolerances was successful.
CV_MEM_NULL	The CVODES memory block was not initialized through a previous call to CVodeCreate.
CV_NO_SENS	The sensitivity allocation function has not been called.

Notes

F2003 Name FCVodeSensEEtolerances

5.2.3 Forward sensitivity nonlinear solver interface functions

As in the pure ODE case, when computing solution sensitivities using forward sensitivitiy analysis CVODES uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §11.3) by default. To specify a different nonlinear solver in CVODES, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine. The user must then attach the SUNNONLINSOL object to CVODES by calling CVodeSetNonlinearSolverSensSim when using the CV_SIMULTANEOUS corrector option, or CVodeSetNonlinearSolver (see §4.5.4) and CVodeSetNonlinearSolverSensStg or CVodeSetNonlinearSolverSensStg1 when using the CV_STAGGERED or CV_STAGGERED1 corrector option respectively, as documented below.

When changing the nonlinear solver in CVODES, CVodeSetNonlinearSolver must be called after CVodeInit; similarly CVodeSetNonlinearSolverSensSim, CVodeSetNonlinearSolverStg, and CVodeSetNonlinearSolverStg1 must be called after CVodeSensInit. If any calls to CVode have been made, then CVODES will need to be reinitialized by calling CVodeReInit to ensure that the nonlinear solver is initialized correctly before any subsequent calls to CVode.

The first argument passed to the routines CVodeSetNonlinearSolverSensSim, CVodeSetNonlinearSolverSensStg, and CVodeSetNonlinearSolverSensStg1 is the CVODES memory pointer returned by CVodeCreate and the second argument is the SUNNONLINSOL object to use for solving the nonlinear systems (2.4) or (2.5). A call to this function attaches the nonlinear solver to the main CVODES integrator.

CVodeSetNonlinearSolverSensSim

Call `flag = CVodeSetNonlinearSolverSensSim(cvode_mem, NLS);`

Description The function CVodeSetNonLinearSolverSensSim attaches a SUNNONLINSOL object (NLS) to CVODES when using the CV_SIMULTANEOUS approach to correct the state and sensitivity variables at the same time.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
NLS	(SUNNonlinearSolver) SUNNONLINSOL object to use for solving nonlinear systems (2.4) or (2.5).

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

CV_SUCCESS	The nonlinear solver was successfully attached.
CV_MEM_NULL	The cvode_mem pointer is NULL.
CV_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 FCVodeSetNonlinearSolverSensSim

CVodeSetNonlinearSolverSensStg

Call `flag = CVodeSetNonlinearSolverSensStg(cvode_mem, NLS);`

Description The function CVodeSetNonLinearSolverSensStg attaches a SUNNONLINSOL object (NLS) to CVODES when using the CV_STAGGERED approach to correct all the sensitivity variables after the correction of the state variables.

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

Return value The return value flag (of type int) is one of
- CV_SUCCESS The nonlinear solver was successfully attached.
- CV_MEM_NULL The cvode_mem pointer is NULL.
- CV_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 CVodeSetNonlinearSolver (see §4.5.4).

F2003 Name FCVodeSetNonlinearSolverSensStg

CVodeSetNonlinearSolverSensStg1

Call flag = CVodeSetNonlinearSolverSensStg1(cvode_mem, NLS);

Description The function CVodeSetNonLinearSolverSensStg1 attaches a SUNNONLINSOL object (NLS) to CVODES when using the CV_STAGGERED1 approach to correct the sensitivity variables one at a time after the correction of the state variables.

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

Return value The return value flag (of type int) is one of
- CV_SUCCESS The nonlinear solver was successfully attached.
- CV_MEM_NULL The cvode_mem pointer is NULL.
- CV_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 CVodeSetNonlinearSolver (see §4.5.4).

F2003 Name FCVodeSetNonlinearSolverSensStg1

5.2.4 CVODES solver function

Even if forward sensitivity analysis was enabled, the call to the main solver function CVode is exactly the same as in §4.5.6. However, in this case the return value flag can also be one of the following:

- CV_SRHSFUNC_FAIL The sensitivity right-hand side function failed in an unrecoverable manner.
- CV_FIRST_SRHSFUNC_ERR The sensitivity right-hand side function failed at the first call.
- CV_REPTD_SRHSFUNC_ERR Convergence tests occurred too many times due to repeated recoverable errors in the sensitivity right-hand side function. This flag will also be returned if the sensitivity right-hand side function had repeated recoverable errors during the estimation of an initial step size.

CV_UNREC_SRHSFUNC_ERR The sensitivity right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the sensitivity right-hand side function fails recoverably after an error test failed while at order one.

5.2.5 Forward sensitivity extraction functions

If forward sensitivity computations have been initialized by a call to CVodeSensInit/CVodeSensInit1, or reinitialized by a call to CVSensReInit, then CVODES computes both a solution and sensitivities at time t. However, CVode will still return only the solution y in yout. Solution sensitivities can be obtained through one of the following functions:

CVodeGetSens

Call `flag = CVodeGetSens(cvode_mem, &tret, yS);`

Description The function CVodeGetSens returns the sensitivity solution vectors after a successful return from CVode.

Arguments
- cvode_mem (void *) pointer to the memory previously allocated by CVodeInit.
- tret (realtype *) the time reached by the solver (output).
- yS (N_Vector *) array of computed forward sensitivity vectors. This vector array must be allocated by the user.

Return value The return value flag of CVodeGetSens is one of:
- CV_SUCCESS CVodeGetSens was successful.
- CV_MEM_NULL cvode_mem was NULL.
- CV_NO_SENS Forward sensitivity analysis was not initialized.
- CV_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 CVode call.

F2003 Name FCVodeGetSens

The function CVodeGetSensDky computes the k-th derivatives of the interpolating polynomials for the sensitivity variables at time t. This function is called by CVodeGetSens with $k = 0$, but may also be called directly by the user.

CVodeGetSensDky

Call `flag = CVodeGetSensDky(cvode_mem, t, k, dkyS);`

Description The function CVodeGetSensDky returns derivatives of the sensitivity solution vectors after a successful return from CVode.

Arguments
- cvode_mem (void *) pointer to the memory previously allocated by CVodeInit.
- 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 CVODES.
- k (int) order of derivatives.
- dkyS (N_Vector *) array of Ns vectors containing the derivatives on output. The space for dkyS must be allocated by the user.

Return value The return value flag of CVodeGetSensDky is one of:
- CV_SUCCESS CVodeGetSensDky succeeded.
- CV_MEM_NULL cvode_mem was NULL.
- CV_NO_SENS Forward sensitivity analysis was not initialized.
- CV_BAD_DKY One of the vectors dkyS is NULL.

CV_BAD_K	k is not in the range $0, 1, ...,$ qlast.
CV_BAD_T	The time t is not in the allowed range.

F2003 Name FCVodeGetSensDky

Forward sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions CVodeGetSens1 and CVodeGetSensDky1, defined as follows:

CVodeGetSens1

Call `flag = CVodeGetSens1(cvode_mem, &tret, is, yS);`

Description The function CVodeGetSens1 returns the is-th sensitivity solution vector after a successful return from CVode.

Arguments

cvode_mem	(void *) pointer to the memory previously allocated by CVodeInit.
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. This vector array must be allocated by the user.

Return value The return value flag of CVodeGetSens1 is one of:

CV_SUCCESS	CVodeGetSens1 was successful.
CV_MEM_NULL	cvode_mem was NULL.
CV_NO_SENS	Forward sensitivity analysis was not initialized.
CV_BAD_IS	The index is is not in the allowed range.
CV_BAD_DKY	yS is NULL.
CV_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 CVode call.

F2003 Name FCVodeGetSens1

CVodeGetSensDky1

Call `flag = CVodeGetSensDky1(cvode_mem, t, k, is, dkyS);`

Description The function CVodeGetSensDky1 returns the k-th derivative of the is-th sensitivity solution vector after a successful return from CVode.

Arguments

cvode_mem	(void *) pointer to the memory previously allocated by CVodeInit.
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 CVODES.
k	(int) order of derivative.
is	(int) specifies the sensitivity derivative vector to be returned ($0 \leq$is$< N_s$).
dkyS	(N_Vector) the vector containing the derivative. The space for dkyS must be allocated by the user.

Return value The return value flag of CVodeGetSensDky1 is one of:

CV_SUCCESS	CVodeGetQuadDky1 succeeded.
CV_MEM_NULL	The pointer to cvode_mem was NULL.
CV_NO_SENS	Forward sensitivity analysis was not initialized.
CV_BAD_DKY	dkyS or one of the vectors dkyS[i] is NULL.
CV_BAD_IS	The index is is not in the allowed range.
CV_BAD_K	k is not in the range $0, 1, ...,$ qlast.
CV_BAD_T	The time t is not in the allowed range.

F2003 Name FCVodeGetSensDky1

5.2.6 Optional inputs for forward sensitivity analysis

Optional input variables that control the computation of sensitivities can be changed from their default values through calls to `CVodeSetSens*` functions. Table 5.1 lists all forward sensitivity optional input functions in CVODES which are described in detail in the remainder of this section.

`CVodeSetSensParams`

Call `flag = CVodeSetSensParams(cvode_mem, p, pbar, plist);`

Description The function `CVodeSetSensParams` specifies problem parameter information for sensitivity calculations.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `p` (`realtype *`) a pointer to the array of real problem parameters used to evaluate $f(t, y, p)$. If non-`NULL`, `p` must point to a field in the user's data structure `user_data` passed to the right-hand side function. (See §5.1).
- `pbar` (`realtype *`) an array of `Ns` positive scaling factors. If non-`NULL`, `pbar` must have all its components > 0.0. (See §5.1).
- `plist` (`int *`) an array of `Ns` non-negative indices to specify which components `p[i]` 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:
- `CV_SUCCESS` The optional value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CV_NO_SENS` Forward sensitivity analysis was not initialized.
- `CV_ILL_INPUT` An argument has an illegal value.

Notes This function must be preceded by a call to `CVodeSensInit` or `CVodeSensInit1`.

F2003 Name `FCVodeSetSensParams`

`CVodeSetSensDQMethod`

Call `flag = CVodeSetSensDQMethod(cvode_mem, DQtype, DQrhomax);`

Description The function `CVodeSetSensDQMethod` specifies the difference quotient strategy in the case in which the right-hand side of the sensitivity equations are to be computed by CVODES.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `DQtype` (`int`) specifies the difference quotient type. Its value can be `CV_CENTERED` or `CV_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 right-hand side.

Return value The return value `flag` (of type `int`) is one of:
- `CV_SUCCESS` The optional value has been successfully set.

Table 5.1: Forward sensitivity optional inputs

Optional input	Routine name	Default
Sensitivity scaling factors	`CVodeSetSensParams`	`NULL`
DQ approximation method	`CVodeSetSensDQMethod`	centered/0.0
Error control strategy	`CVodeSetSensErrCon`	`SUNFALSE`
Maximum no. of nonlinear iterations	`CVodeSetSensMaxNonlinIters`	3

CV_MEM_NULL The cvode_mem pointer is NULL.

CV_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 $\geq$ 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 §2.6 for more details.

The default value are DQtype=CV_CENTERED and DQrhomax= 0.0.

F2003 Name FCVodeSetSensDQMethod

CVodeSetSensErrCon

Call `flag = CVodeSetSensErrCon(cvode_mem, errconS);`

Description The function CVodeSetSensErrCon specifies the error control strategy for sensitivity variables.

Arguments cvode_mem (void *) pointer to the CVODES memory block.

errconS (booleantype) specifies whether sensitivity variables are to be included (SUNTRUE) or not (SUNFALSE) in the error control mechanism.

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

CV_SUCCESS The optional value has been successfully set.

CV_MEM_NULL The cvode_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 FCVodeSetSensErrCon

CVodeSetSensMaxNonlinIters

Call `flag = CVodeSetSensMaxNonlinIters(cvode_mem, maxcorS);`

Description The function CVodeSetSensMaxNonlinIters specifies the maximum number of nonlinear solver iterations for sensitivity variables per step.

Arguments cvode_mem (void *) pointer to the CVODES 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:

CV_SUCCESS The optional value has been successfully set.

CV_MEM_NULL The cvode_mem pointer is NULL.

CV_MEM_FAIL The SUNNONLINSOL module is NULL.

Notes The default value is 3.

F2003 Name FCVodeSetSensMaxNonlinIters

5.2.7 Optional outputs for forward sensitivity analysis

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.

`CVodeGetSensNumRhsEvals`

Call `flag = CVodeGetSensNumRhsEvals(cvode_mem, &nfSevals);`

Description The function `CVodeGetSensNumRhsEvals` returns the number of calls to the sensitivity right-hand side function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nfSevals` (`long int`) number of calls to the sensitivity right-hand side function.

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_NO_SENS` Forward sensitivity analysis was not initialized.

Notes In order to accommodate any of the three possible sensitivity solution methods, the default internal finite difference quotient functions evaluate the sensitivity right-hand sides one at a time. Therefore, `nfSevals` will always be a multiple of the number of sensitivity parameters (the same as the case in which the user supplies a routine of type `CVSensRhs1Fn`).

F2003 Name `FCVodeGetSensNumRhsEvals`

`CVodeGetNumRhsEvalsSens`

Call `flag = CVodeGetNumRhsEvalsSens(cvode_mem, &nfevalsS);`

Description The function `CVodeGetNumRhsEvalsSEns` returns the number of calls to the user's right-hand side function due to the internal finite difference approximation of the sensitivity right-hand sides.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nfevalsS` (`long int`) number of calls to the user's ODE right-hand side function for the evaluation of sensitivity right-hand sides.

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_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 right-hand sides.

F2003 Name `FCVodeGetNumRhsEvalsSens`

Table 5.2: Forward sensitivity optional outputs

Optional output	**Routine name**
No. of calls to sensitivity r.h.s. function	`CVodeGetSensNumRhsEvals`
No. of calls to r.h.s. function for sensitivity	`CVodeGetNumRhsEvalsSens`
No. of sensitivity local error test failures	`CVodeGetSensNumErrTestFails`
No. of calls to lin. solv. setup routine for sens.	`CVodeGetSensNumLinSolvSetups`
Error weight vector for sensitivity variables	`CVodeGetSensErrWeights`
No. of sens. nonlinear solver iterations	`CVodeGetSensNumNonlinSolvIters`
No. of sens. convergence failures	`CVodeGetSensNumNonlinSolvConvFails`
No. of staggered nonlinear solver iterations	`CVodeGetStgrSensNumNonlinSolvIters`
No. of staggered convergence failures	`CVodeGetStgrSensNumNonlinSolvConvFails`

`CVodeGetSensNumErrTestFails`

Call `flag = CVodeGetSensNumErrTestFails(cvode_mem, &nSetfails);`

Description The function `CVodeGetSensNumErrTestFails` returns the number of local error test failures for the sensitivity variables that have occurred.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nSetfails` (`long int`) number of error test failures.

Return value The return value `flag` (of type `int`) is one of:
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_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 `CVodeSetSensErrCon` in §5.2.6). Even in that case, this counter is not incremented if the `ism`=`CV_SIMULTANEOUS` sensitivity solution method has been used.

F2003 Name `FCVodeGetSensNumErrTestFails`

`CVodeGetSensNumLinSolvSetups`

Call `flag = CVodeGetSensNumLinSolvSetups(cvode_mem, &nlinsetupsS);`

Description The function `CVodeGetSensNumLinSolvSetups` returns the number of calls to the linear solver setup function due to forward sensitivity calculations.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:
`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if a nonlinear solver requiring a linear solve has been used and if either the `ism` = `CV_STAGGERED` or the `ism` = `CV_STAGGERED1` sensitivity solution method has been specified (see §5.2.1).

F2003 Name `FCVodeGetSensNumLinSolvSetups`

`CVodeGetSensStats`

Call
```
flag = CVodeGetSensStats(cvode_mem, &nfSevals, &nfevalsS, &nSetfails,
                         &nSetfails, &nlinsetupsS);
```

Description The function `CVodeGetSensStats` returns all of the above sensitivity-related solver statistics as a group.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nfSevals` (`long int`) number of calls to the sensitivity right-hand side function.
`nfevalsS` (`long int`) number of calls to the ODE right-hand side function for sensitivity evaluations.
`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:
`CV_SUCCESS` The optional output values have been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

F2003 Name `FCVodeGetSensStats`

`CVodeGetSensErrWeights`

Call `flag = CVodeGetSensErrWeights(cvode_mem, eSweight);`

Description The function `CVodeGetSensErrWeights` returns the sensitivity error weight vectors at the current time. These are the reciprocals of the W_i of (2.8) for the sensitivity variables.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`eSweight` (`N_Vector *`) pointer to the array of error weight vectors.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

Notes The user must allocate memory for `eweightS`.

F2003 Name `FCVodeGetSensErrWeights`

`CVodeGetSensNumNonlinSolvIters`

Call `flag = CVodeGetSensNumNonlinSolvIters(cvode_mem, &nSniters);`

Description The function `CVodeGetSensNumNonlinSolvIters` returns the number of nonlinear iterations performed for sensitivity calculations.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nSniters` (`long int`) number of nonlinear iterations performed.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS` Forward sensitivity analysis was not initialized.
`CV_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

Notes This counter is incremented only if `ism` was `CV_STAGGERED` or `CV_STAGGERED1` (see §5.2.1).

In the `CV_STAGGERED1` case, the value of `nSniters` is the sum of the number of nonlinear iterations performed for each sensitivity equation. These individual counters can be obtained through a call to `CVodeGetStgrSensNumNonlinSolvIters` (see below).

F2003 Name `FCVodeGetSensNumNonlinSolvIters`

`CVodeGetSensNumNonlinSolvConvFails`

Call `flag = CVodeGetSensNumNonlinSolvConvFails(cvode_mem, &nSncfails);`

Description The function `CVodeGetSensNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred for sensitivity calculations.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`nSncfails` (`long int`) number of nonlinear convergence failures.

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

`CV_SUCCESS` The optional output value has been successfully set.
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

Notes This counter is incremented only if `ism` was `CV_STAGGERED` or `CV_STAGGERED1` (see §5.2.1).

In the `CV_STAGGERED1` case, the value of `nSncfails` is the sum of the number of nonlinear convergence failures that occurred for each sensitivity equation. These individual counters can be obtained through a call to `CVodeGetStgrSensNumNonlinConvFails` (see below).

F2003 Name `FCVodeGetSensNumNonlinSolvConvFails`

`CVodeGetSensNonlinSolvStats`

Call `flag = CVodeGetSensNonlinSolvStats(cvode_mem, &nSniters, &nSncfails);`

Description The function `CVodeGetSensNonlinSolvStats` returns the sensitivity-related nonlinear solver statistics as a group.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS` The optional output values have been successfully set.

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_NO_SENS` Forward sensitivity analysis was not initialized.

`CV_MEM_FAIL` The SUNNONLINSOL module is `NULL`.

F2003 Name `FCVodeGetSensNonlinSolvStats`

`CVodeGetStgrSensNumNonlinSolvIters`

Call `flag = CVodeGetStgrSensNumNonlinSolvIters(cvode_mem, nSTGR1niters);`

Description The function `CVodeGetStgrSensNumNonlinSolvIters` returns the number of nonlinear iterations performed for each sensitivity equation separately, in the `CV_STAGGERED1` case.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nSTGR1niters` (`long int *`) an array (of dimension `Ns`) which will be set with the number of nonlinear iterations performed for each sensitivity system individually.

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CV_NO_SENS` Forward sensitivity analysis was not initialized.

Notes The user must allocate space for `nSTGR1niters`.

F2003 Name `FCVodeGetStgrSensNumNonlinSolvIters`

`CVodeGetStgrSensNumNonlinSolvConvFails`

Call `flag = CVodeGetStgrSensNumNonlinSolvConvFails(cvode_mem, nSTGR1ncfails);`

Description The function `CVodeGetStgrSensNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred for each sensitivity equation separately, in the `CV_STAGGERED1` case.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`nSTGR1ncfails` (`long int *`) an array (of dimension `Ns`) which will be set with the number of nonlinear convergence failures for each sensitivity system individually.

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

`CV_SUCCESS`	The optional output value has been successfully set.
`CV_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS`	Forward sensitivity analysis was not initialized.

Notes The user must allocate space for `nSTGR1ncfails`.

F2003 Name `FCVodeGetStgrSensNumNonlinSolvConvFails`

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 CVODES for forward sensitivity analysis, the user has the option of providing a routine that calculates the right-hand side of the sensitivity equations (2.12).

By default, CVODES uses difference quotient approximation routines for the right-hand sides of the sensitivity equations. However, CVODES allows the option for user-defined sensitivity right-hand side routines (which also provides a mechanism for interfacing CVODES to routines generated by automatic differentiation).

5.3.1 Sensitivity equations right-hand side (all at once)

If the `CV_SIMULTANEOUS` or `CV_STAGGERED` approach was selected in the call to `CVodeSensInit` or `CVodeSensInit1`, the user may provide the right-hand sides of the sensitivity equations (2.12), for all sensitivity parameters at once, through a function of type `CVSensRhsFn` defined by:

`CVSensRhsFn`

Definition
```
typedef int (*CVSensRhsFn)(int Ns, realtype t,
                           N_Vector y, N_Vector ydot,
                           N_Vector *yS, N_Vector *ySdot,
                           void *user_data,
                           N_Vector tmp1, N_Vector tmp2);
```

Purpose This function computes the sensitivity right-hand side for all sensitivity equations at once. It must compute the vectors $(\partial f/\partial y)s_i(t)+(\partial f/\partial p_i)$ and store them in `ySdot[i]`.

Arguments

`Ns`	is the number of sensitivities.
`t`	is the current value of the independent variable.
`y`	is the current value of the state vector, $y(t)$.
`ydot`	is the current value of the right-hand side of the state equations.
`yS`	contains the current values of the sensitivity vectors.
`ySdot`	is the output of `CVSensRhsFn`. On exit it must contain the sensitivity right-hand side vectors.
`user_data`	is a pointer to user data, the same as the `user_data` parameter passed to `CVodeSetUserData`.
`tmp1` `tmp2`	are `N_Vector`s of length N which can be used as temporary storage.

Return value A `CVSensRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CV_SRHSFUNC_FAIL` is returned).

Notes A sensitivity right-hand side function of type `CVSensRhsFn` is not compatible with the `CV_STAGGERED1` approach.

Allocation of memory for `ySdot` is handled within CVODES.

There are two situations in which recovery is not possible even if CVSensRhsFn function returns a recoverable error flag. One is when this occurs at the very first call to the CVSensRhsFn (in which case CVODES returns CV_FIRST_SRHSFUNC_ERR). The other is when a recoverable error is reported by CVSensRhsFn after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns CV_UNREC_SRHSFUNC_ERR).

5.3.2 Sensitivity equations right-hand side (one at a time)

Alternatively, the user may provide the sensitivity right-hand sides, one sensitivity parameter at a time, through a function of type CVSensRhs1Fn. Note that a sensitivity right-hand side function of type CVSensRhs1Fn is compatible with any valid value of the argument ism to CVodeSensInit and CVodeSensInit1, and is *required* if ism = CV_STAGGERED1 in the call to CVodeSensInit1. The type CVSensRhs1Fn is defined by

CVSensRhs1Fn

Definition
```
typedef int (*CVSensRhs1Fn)(int Ns, realtype t,
                            N_Vector y, N_Vector ydot,
                            int iS, N_Vector yS, N_Vector ySdot,
                            void *user_data,
                            N_Vector tmp1, N_Vector tmp2);
```

Purpose This function computes the sensitivity right-hand side for one sensitivity equation at a time. It must compute the vector $(\partial f/\partial y)s_i(t) + (\partial f/\partial p_i)$ for $i =$ iS and store it in ySdot.

Arguments
- Ns is the number of sensitivities.
- t is the current value of the independent variable.
- y is the current value of the state vector, $y(t)$.
- ydot is the current value of the right-hand side of the state equations.
- iS is the index of the parameter for which the sensitivity right-hand side must be computed ($0 \le$ iS $<$ Ns).
- yS contains the current value of the iS-th sensitivity vector.
- ySdot is the output of CVSensRhs1Fn. On exit it must contain the iS-th sensitivity right-hand side vector.
- user_data is a pointer to user data, the same as the user_data parameter passed to CVodeSetUserData.
- tmp1
- tmp2 are N_Vectors of length N which can be used as temporary storage.

Return value A CVSensRhs1Fn should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and CV_SRHSFUNC_FAIL is returned).

Notes Allocation of memory for ySdot is handled within CVODES.

There are two situations in which recovery is not possible even if CVSensRhs1Fn function returns a recoverable error flag. One is when this occurs at the very first call to the CVSensRhs1Fn (in which case CVODES returns CV_FIRST_SRHSFUNC_ERR). The other is when a recoverable error is reported by CVSensRhs1Fn after an error test failure, while the linear multistep method order equal to 1 (in which case CVODES returns CV_UNREC_SRHSFUNC_ERR).

5.4 Integration of quadrature equations depending on forward sensitivities

CVODES 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.

1. **Initialize parallel or multi-threaded environment, if appropriate**
2. **Set problem dimensions etc.**
3. **Set vectors of initial values**
4. **Create CVODES object**
5. **Initialize CVODES 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 `CVodeQuadSensInit` 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 `CVodeSetQuadSensErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `CVodeQuadSens*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 `CVodeGetQuadSens`, `CVodeGetQuadSens1`, `CVodeGetQuadSensDky` or `CVodeGetQuadSensDky1` 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 `CVodeGetQuadSens*` functions to obtain desired 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: `CVodeQuadSensInit` (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 `CVodeQuadSensInit` activates integration of quadrature equations depending on sensitivities and allocates internal memory related to these calculations. If `rhsQS` is input as `NULL`, then CVODES uses an internal function that computes difference quotient approximations to the functions $\bar{q}_i = q_y s_i + q_{p_i}$, in the notation of (2.10). The form of the call to this function is as follows:

`CVodeQuadSensInit`

Call `flag = CVodeQuadSensInit(cvode_mem, rhsQS, yQS0);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.

`rhsQS` (`CVQuadSensRhsFn`) 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:

`CV_SUCCESS` The call to `CVodeQuadSensInit` was successful.

`CVODE_MEM_NULL` The CVODES memory was not initialized by a prior call to `CVodeCreate`.

`CVODE_MEM_FAIL` A memory allocation request failed.

`CV_NO_SENS` The sensitivities were not initialized by a prior call to `CVodeSensInit` or `CVodeSensInit1`.

`CV_ILL_INPUT` The parameter `yQS0` is `NULL`.

Notes Before calling `CVodeQuadSensInit`, the user must enable the sensitivites by calling `CVodeSensInit` or `CVodeSensInit1`.

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

F2003 Name `FCVodeQuadSensInit`

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 `CVodeQuadSensSVtolerances` is called: `lenrw` = `lenrw` +$N_q N_s$

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

- Base value: `leniw` = `leniw` + (`maxord`+5)N_q
- If `CVodeQuadSensSVtolerances` is called: `leniw` = `leniw` +$N_q N_s$

The function `CVodeQuadSensReInit`, useful during the solution of a sequence of problems of same size, reinitializes quadrature-related internal memory and must follow a call to `CVodeQuadSensInit`. The number `Nq` of quadratures as well as the number `Ns` of sensitivities are assumed to be unchanged from the prior call to `CVodeQuadSensInit`. The call to the `CVodeQuadSensReInit` function has the form:

`CVodeQuadSensReInit`

Call `flag = CVodeQuadSensReInit(cvode_mem, yQS0);`

Description The function `CVodeQuadSensReInit` provides required problem specifications and reinitializes the sensitivity-dependent quadrature integration.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS` The call to `CVodeQuadSensReInit` was successful.

`CVODE_MEM_NULL` The CVODES memory was not initialized by a prior call to `CVodeCreate`.

`CV_NO_SENS` Memory space for the sensitivity calculation was not allocated by a prior call to `CVodeSensInit` or `CVodeSensInit1`.

`CV_NO_QUADSENS` Memory space for the sensitivity quadratures integration was not allocated by a prior call to `CVodeQuadSensInit`.

`CV_ILL_INPUT` The parameter `yQS0` is `NULL`.

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

F2003 Name `FCVodeQuadSensReInit`

`CVodeQuadSensFree`

Call `CVodeQuadSensFree(cvode_mem);`

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

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

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

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

F2003 Name `FCVodeQuadSensFree`

5.4.2 CVODES solver function

Even if quadrature integration was enabled, the call to the main solver function `CVode` is exactly the same as in §4.5.6. However, in this case the return value `flag` can also be one of the following:

`CV_QSRHSFUNC_ERR` The sensitivity quadrature right-hand side function failed in an unrecoverable manner.

`CV_FIRST_QSRHSFUNC_ERR` The sensitivity quadrature right-hand side function failed at the first call.

`CV_REPTD_QSRHSFUNC_ERR` Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. This flag 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 `CVodeQuadSensInit`, or reinitialized by a call to `CVodeQuadSensReInit`, then CVODES computes a solution, sensitivity vectors, and quadratures depending on sensitivities at time `t`. However, `CVode` will still return only the solution y. Sensitivity-dependent quadratures can be obtained using one of the following functions:

`CVodeGetQuadSens`

Call `flag = CVodeGetQuadSens(cvode_mem, &tret, yQS);`

Description The function `CVodeGetQuadSens` returns the quadrature sensitivities solution vectors after a successful return from `CVode`.

Arguments `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.

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

`yQS` (`N_Vector *`) array of `Ns` computed sensitivity-dependent quadrature vectors. This vector array must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuadSens` is one of:

`CV_SUCCESS`	`CVodeGetQuadSens` was successful.
`CVODE_MEM_NULL`	`cvode_mem` was NULL.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_BAD_DKY`	`yQS` or one of the `yQS[i]` is `NULL`.

F2003 Name `FCVodeGetQuadSens`

The function `CVodeGetQuadSensDky` computes the `k`-th derivatives of the interpolating polynomials for the sensitivity-dependent quadrature variables at time `t`. This function is called by `CVodeGetQuadSens` with `k = 0`, but may also be called directly by the user.

`CVodeGetQuadSensDky`

Call `flag = CVodeGetQuadSensDky(cvode_mem, t, k, dkyQS);`

Description The function `CVodeGetQuadSensDky` returns derivatives of the quadrature sensitivities solution vectors after a successful return from `CVode`.

Arguments
`cvode_mem`	(`void *`) pointer to the memory previously allocated by `CVodeInit`.
`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 CVODES.
`k`	(`int`) order of the requested derivative.
`dkyQS`	(`N_Vector *`) array of `Ns` the vector containing the derivatives on output. This vector array must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuadSensDky` is one of:
`CV_SUCCESS`	`CVodeGetQuadSensDky` succeeded.
`CVODE_MEM_NULL`	The pointer to `cvode_mem` was `NULL`.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_BAD_DKY`	`dkyQS` or one of the vectors `dkyQS[i]` is `NULL`.
`CV_BAD_K`	`k` is not in the range $0, 1, ...,$ `qlast`.
`CV_BAD_T`	The time `t` is not in the allowed range.

F2003 Name `FCVodeGetQuadSensDky`

Quadrature sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions `CVodeGetQuadSens1` and `CVodeGetQuadSensDky1`, defined as follows:

`CVodeGetQuadSens1`

Call `flag = CVodeGetQuadSens1(cvode_mem, &tret, is, yQS);`

Description The function `CVodeGetQuadSens1` returns the `is`-th sensitivity of quadratures after a successful return from `CVode`.

Arguments
`cvode_mem`	(`void *`) pointer to the memory previously allocated by `CVodeInit`.
`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 array must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuadSens1` is one of:
`CV_SUCCESS`	`CVodeGetQuadSens1` was successful.
`CVODE_MEM_NULL`	`cvode_mem` was `NULL`.
`CV_NO_SENS`	Forward sensitivity analysis was not initialized.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_BAD_IS`	The index `is` is not in the allowed range.
`CV_BAD_DKY`	`yQS` is `NULL`.

F2003 Name `FCVodeGetQuadSens1`

`CVodeGetQuadSensDky1`

Call `flag = CVodeGetQuadSensDky1(cvode_mem, t, k, is, dkyQS);`

Description The function `CVodeGetQuadSensDky1` returns the `k`-th derivative of the `is`-th sensitivity solution vector after a successful return from `CVode`.

Arguments `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.

`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 CVODES.
`k`	(`int`) order of derivative.
`is`	(`int`) specifies the sensitivity derivative vector to be returned ($0 \leq$`is`$< N_s$).
`dkyQS`	(`N_Vector`) the vector containing the derivative on output. The space for `dkyQS` must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuadSensDky1` is one of:

`CV_SUCCESS`	`CVodeGetQuadDky1` succeeded.
`CVODE_MEM_NULL`	`cvode_mem` was `NULL`.
`CV_NO_SENS`	Forward sensitivity analysis was not initialized.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_BAD_DKY`	`dkyQS` is `NULL`.
`CV_BAD_IS`	The index `is` is not in the allowed range.
`CV_BAD_K`	`k` is not in the range $0, 1, ...,$ `qlast`.
`CV_BAD_T`	The time `t` is not in the allowed range.

F2003 Name `FCVodeGetQuadSensDky1`

5.4.4 Optional inputs for sensitivity-dependent quadrature integration

CVODES provides the following optional input functions to control the integration of sensitivity-dependent quadrature equations.

`CVodeSetQuadSensErrCon`

Call `flag = CVodeSetQuadSensErrCon(cvode_mem, errconQS)`

Description The function `CVodeSetQuadSensErrCon` specifies whether or not the quadrature variables are to be used in the step size control mechanism. If they are, the user must call one of the functions `CVodeQuadSensSStolerances`, `CVodeQuadSensSVtolerances`, or `CVodeQuadSensEEtolerances` to specify the integration tolerances for the quadrature variables.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

`errconQS` (`booleantype`) specifies whether sensitivity quadrature variables are to be included (`SUNTRUE`) or not (`SUNFALSE`) in the error control mechanism.

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

`CV_SUCCESS`	The optional value has been successfully set.
`CVODE_MEM_NULL`	`cvode_mem` is `NULL`.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.

Notes By default, `errconQS` is set to `SUNFALSE`.

It is illegal to call `CVodeSetQuadSensErrCon` before a call to `CVodeQuadSensInit`.

F2003 Name `FCVodeSetQuadSensErrCon`

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.

`CVodeQuadSensSStolerances`

Call `flag = CVodeQuadSensSVtolerances(cvode_mem, reltolQS, abstolQS);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional value has been successfully set.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FCVodeQuadSensSStolerances`

`CVodeQuadSensSVtolerances`

Call `flag = CVodeQuadSensSVtolerances(cvode_mem, reltolQS, abstolQS);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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 abstolS[is]` specifies the vector tolerances for `is`-th quadrature sensitivity.

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

`CV_SUCCESS`	The optional value has been successfully set.
`CV_NO_QUAD`	Quadrature integration was not initialized.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.
`CV_ILL_INPUT`	One of the input tolerances was negative.

F2003 Name `FCVodeQuadSensSVtolerances`

`CVodeQuadSensEEtolerances`

Call `flag = CVodeQuadSensEEtolerances(cvode_mem);`

Description A call to the function `CVodeQuadSensEEtolerances` specifies that the tolerances for the sensitivity-dependent quadratures should be estimated from those provided for the pure quadrature variables.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.

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

`CV_SUCCESS`	The optional value has been successfully set.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_SENS`	Sensitivities were not activated.
`CV_NO_QUADSENS`	Quadratures depending on the sensitivities were not activated.

Notes When `CVodeQuadSensEEtolerances` is used, before calling `CVode`, 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 `FCVodeQuadSensEEtolerances`

5.4.5 Optional outputs for sensitivity-dependent quadrature integration

CVODES provides the following functions that can be used to obtain solver performance information related to quadrature integration.

`CVodeGetQuadSensNumRhsEvals`

Call `flag = CVodeGetQuadSensNumRhsEvals(cvode_mem, &nrhsQSevals);`

Description The function `CVodeGetQuadSensNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional output value has been successfully set.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_QUADSENS`	Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadSensNumRhsEvals`

`CVodeGetQuadSensNumErrTestFails`

Call `flag = CVodeGetQuadSensNumErrTestFails(cvode_mem, &nQSetfails);`

Description The function `CVodeGetQuadSensNumErrTestFails` returns the number of local error test failures due to quadrature variables.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional output value has been successfully set.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_NO_QUADSENS`	Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadSensNumErrTestFails`

`CVodeGetQuadSensErrWeights`

Call `flag = CVodeGetQuadSensErrWeights(cvode_mem, eQSweight);`

Description The function `CVodeGetQuadSensErrWeights` returns the quadrature error weights at the current time.

Arguments `cvode_mem` (`void *`) pointer to the CVODES 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:

`CV_SUCCESS`	The optional output value has been successfully set.
`CVODE_MEM_NULL`	The `cvode_mem` pointer is `NULL`.
`CV_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 `CVodeSetQuadSensErrCon` with `errconQS = SUNTRUE`), then this function does not set the `eQSweight` array.

F2003 Name `FCVodeGetQuadSensErrWeights`

`CVodeGetQuadSensStats`

Call `flag = CVodeGetQuadSensStats(cvode_mem, &nrhsQSevals, &nQSetfails);`

Description The function `CVodeGetQuadSensStats` returns the CVODES integrator statistics as a group.

Arguments
`cvode_mem`	(`void *`) pointer to the CVODES 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
`CV_SUCCESS`	the optional output values have been successfully set.
`CVODE_MEM_NULL`	the `cvode_mem` pointer is `NULL`.
`CV_NO_QUADSENS`	Sensitivity-dependent quadrature integration has not been initialized.

F2003 Name `FCVodeGetQuadSensStats`

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 those quadrature equations. For the sensitivities of quadratures (2.10) with integrand q, the appropriate right-hand side functions are given by: $\bar{q}_i = q_y s_i + q_{p_i}$. This user function must be of type `CVQuadSensRhsFn` defined as follows:

`CVQuadSensRhsFn`

Definition
```
typedef int (*CVQuadSensRhsFn)(int Ns, realtype t, N_Vector y,
                               N_Vector yS, N_Vector yQdot,
                               N_Vector *rhsvalQS, void *user_data,
                               N_Vector tmp1, N_Vector tmp2)
```

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.
`y`	is the current value of the dependent variable vector, $y(t)$.
`yS`	is an array of `Ns` variables of type `N_Vector` containing the dependent sensitivity vectors s_i.
`yQdot`	is the current value of the quadrature right-hand side, q.
`rhsvalQS`	array of `Ns` vectors to contain the right-hand sides.
`user_data`	is the `user_data` pointer passed to `CVodeSetUserData`.
`tmp1`	
`tmp2`	are `N_Vectors` which can be used as temporary storage.

Return value A `CVQuadSensRhsFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CV_QRHS_FAIL` is returned).

Notes

Allocation of memory for `rhsvalQS` is automatically handled within CVODES.

Here `y` is of type `N_Vector` and `yS` is a pointer 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 CVODES do not perform any consistency checks with respect to their `N_Vector` arguments (see §8.3 and §8.4).

There are two situations in which recovery is not possible even if `CVQuadSensRhsFn` function returns a recoverable error flag. One is when this occurs at the very first call to the `CVQuadSensRhsFn` (in which case CVODES returns `CV_FIRST_QSRHSFUNC_ERR`). The other is when a recoverable error is reported by `CVQuadSensRhsFn` after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns `CV_UNREC_QSRHSFUNC_ERR`).

5.5 Note on using partial error control

For some problems, when sensitivities are excluded from the error control test, the behavior of CVODES 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. A comparison of the solver diagnostics reported for `cvsdenx` and the second run of the `cvsfwddenx` example in [50] indicates that this may not always be the case.

The short explanation of this behavior is that the step size selection implemented by the error control mechanism in CVODES 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 `CVodeSetSensErrCon`), the sensitivity variables are included in the convergence tests of the nonlinear solver.

When using the simultaneous corrector method (§2.6), 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. After all, in this case (`ism = CV_STAGGERED` or `CV_STAGGERED1` in the call to `CVodeSensInit`/`CVodeSensInit1`), 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, CVODES 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, CVODES may trigger a call to the linear solver's setup routine which typically involves reevaluation of Jacobian information (Jacobian approximation in the case of CVDENSE and CVBAND, 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 ODEs 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 CVODES 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 final 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 CVODES. 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 CVODES for Adjoint Sensitivity Analysis

This chapter describes the use of CVODES to compute sensitivities of derived functions using adjoint sensitivity analysis. As mentioned before, the adjoint sensitivity module of CVODES provides the infrastructure for integrating backward in time any system of ODEs that depends on the solution of the original IVP, by providing various interfaces to the main CVODES 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 ODEs that are integrated backward in time. The backward problem can be the adjoint problem (2.20) or (2.23), and can be augmented with some quadrature differential equations.

CVODES 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 CVODES. 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 8, 9, 10, and 11 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 `cvodes.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, if appropriate**

Forward problem

3. **Set problem dimensions etc. for the forward problem**

4. **Set initial conditions for the forward problem**
5. **Create CVODES object for the forward problem**
6. **Initialize CVODES for the forward problem**
7. **Specify integration tolerances for forward problem**
8. **Create matrix object for the forward problem**
9. **Create linear solver object for the forward problem**
10. **Set linear solver optional inputs for the forward problem**
11. **Attach linear solver module for the forward problem**
12. **Set optional inputs for the forward problem**
13. **Create nonlinear solver object 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 `CVodeQuadInit` and/or `CVodeQuadSensInit`.**
17. **Initialize forward sensitivity problem**
18. **Specify rootfinding**
19. **Allocate space for the adjoint computation**

    Call `CVodeAdjInit()` 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. `CVodeAdjInit` also specifies the type of interpolation used (see §2.7.1).

20. **Integrate forward problem**

    Call `CVodeF`, a wrapper for the CVODES main integration function `CVode`, either in `CV_NORMAL` mode to the time `tout` or in `CV_ONE_STEP` mode inside a loop (if intermediate solutions of the forward problem are desired (see §6.2.2)). The final value of `tret` is then the maximum allowable value for the endpoint T of the backward problem.

Backward problem(s)

21. **Set problem dimensions etc. for the backward problem**

    This generally includes the backward problem vector length `NB`, 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 vector `yB0` at which the backward problem starts.

23. **Create the backward problem**

    Call `CVodeCreateB`, a wrapper for `CVodeCreate`, to create the CVODES memory block for the new backward problem. Unlike `CVodeCreate`, the function `CVodeCreateB` does not return a pointer to the newly created memory block (see §6.2.3). Instead, this pointer is attached to the internal adjoint memory block (created by `CVodeAdjInit`) 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 `CVodeInitB` (or `CVodeInitBS`, when the backward problem depends on the forward sensitivities). The two functions are actually wrappers for `CVodeInit` and allocate internal memory, specify problem data, and initialize CVODES at `tB0` for the backward problem (see §6.2.3).

25. **Specify integration tolerances for backward problem**

    Call `CVodeSStolerancesB(...)` or `CVodeSVtolerancesB(...)` to specify a scalar relative tolerance and scalar absolute tolerance or scalar relative tolerance and a vector of absolute tolerances, respectively. The functions are wrappers for `CVodeSStolerances` and `CVodeSVtolerances`, but they require an extra argument `which`, the identifier of the backward problem returned by `CVodeCreateB`. See §6.2.4 for more information.

26. **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.

    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.

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

27. **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.

    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 10.

    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.

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

    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 10 for details.

29. **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 CVLS linear solver interface by attaching the linear solver

object (and matrix object, if applicable) with the call (for details see §4.5.3):

```
ier = CVodeSetLinearSolverB(...);
```

Alternately, if the CVODES-specific diagonal linear solver module, CVDIAG, is desired, initialize the linear solver module and attach it to CVODES with the call

```
ier = CVDiagB(...);
```

30. **Set optional inputs for the backward problem**

    Call `CVodeSet*B` functions to change from their default values any optional inputs that control the behavior of CVODES. Unlike their counterparts for the forward problem, these functions take an extra argument `which`, the identifier of the backward problem returned by `CVodeCreateB` (see §6.2.8).

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 11 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 = CVodeSetNonlinearSolverB(cvode_mem, NLSB);` (see §4.5.4 for details).

33. **Initialize quadrature calculation**

    If additional quadrature equations must be evaluated, call `CVodeQuadInitB` or `CVodeQuadInitBS` (if quadrature depends also on the forward sensitivities) as shown in §6.2.10.1. These functions are wrappers around `CVodeQuadInit` and can be used to initialize and allocate memory for quadrature integration. Optionally, call `CVodeSetQuad*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 `CVodeB`, a second wrapper around the CVODES main integration function `CVode`, to integrate the backward problem from `tB0` (see §6.2.6). This function can be called either in `CV_NORMAL` or `CV_ONE_STEP` mode. Typically, `CVodeB` will be called in `CV_NORMAL` mode with an end time equal to the initial time t_0 of the forward problem.

35. **Extract quadrature variables**

    If applicable, call `CVodeGetQuadB`, a wrapper around `CVodeGetQuad`, to extract the values of the quadrature variables at the time returned by the last call to `CVodeB`. See §6.2.10.2.

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 `CVodeFree` to free the CVODES memory block for the forward problem. If one or more additional Adjoint Sensitivity Analyses are to be done for this problem, a call to `CVodeAdjFree` (see §6.2.1) may be made to free and deallocate memory allocated for the backward problems, followed by a call to `CVodeAdjInit`.

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 CVODES was motivated by the desire to keep it as close as possible in look and feel to the one for ODE 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 ODEs, 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 `CVodeCreateB` 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 `CVodeF`, memory for the combined forward-backward problem must be allocated by a call to the function `CVodeAdjInit`. The form of the call to this function is

`CVodeAdjInit`

Call `flag = CVodeAdjInit(cvode_mem, Nd, interpType);`

Description The function `CVodeAdjInit` updates CVODES memory block by allocating the internal memory needed for backward integration. Space is allocated for the `Nd` $= N_d$ interpolation data points, and a linked list of checkpoints is initialized.

Arguments
- `cvode_mem` (`void *`) is the pointer to the CVODES memory block returned by a previous call to `CVodeCreate`.
- `Nd` (`long int`) is the number of integration steps between two consecutive checkpoints.
- `interpType` (`int`) specifies the type of interpolation used and can be `CV_POLYNOMIAL` or `CV_HERMITE`, indicating variable-degree polynomial and cubic Hermite interpolation, respectively (see §2.7.1).

Return value The return value `flag` (of type `int`) is one of:
- `CV_SUCCESS` `CVodeAdjInit` was successful.
- `CV_MEM_FAIL` A memory allocation request has failed.
- `CV_MEM_NULL` `cvode_mem` was NULL.
- `CV_ILL_INPUT` One of the parameters was invalid: `Nd` was not positive or `interpType` is not one of the `CV_POLYNOMIAL` or `CV_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. `CVodeAdjInit` attempts to allocate space for (2`Nd`+3) variables of type `N_Vector`.

If an error occurred, `CVodeAdjInit` also sends a message to the error handler function.

F2003 Name `FCVodeAdjInit`

`CVodeAdjReInit`

Call `flag = CVodeAdjReInit(cvode_mem);`

Description The function `CVodeAdjReInit` reinitializes the CVODES memory block for ASA, assuming that the number of steps between check points and the type of interpolation remain unchanged.

Arguments
- `cvode_mem` (`void *`) is the pointer to the CVODES memory block returned by a previous call to `CVodeCreate`.

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

CV_SUCCESS	CVodeAdjReInit was successful.
CV_MEM_NULL	cvode_mem was NULL.
CV_NO_ADJ	The function CVodeAdjInit 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 CVodeCreateB. If a new list of backward problems is also needed, then free the adjoint memory (by calling CVodeAdjFree) and reinitialize ASA with CVodeAdjInit.

The CVODES memory for the forward and backward problems can be reinitialized separately by calling CVodeReInit and CVodeReInitB, respectively.

F2003 Name FCVodeAdjReInit

CVodeAdjFree

Call `CVodeAdjFree(cvode_mem);`

Description The function CVodeAdjFree frees the memory related to backward integration allocated by a previous call to CVodeAdjInit.

Arguments The only argument is the CVODES memory block pointer returned by a previous call to CVodeCreate.

Return value The function CVodeAdjFree has no return value.

Notes This function frees all memory allocated by CVodeAdjInit. This includes workspace memory, the linked list of checkpoints, memory for the interpolation data, as well as the CVODES memory for the backward integration phase. Unless one or more further calls to CVodeAdjInit are to be made, CVodeAdjFree should not be called by the user, as it is invoked automatically by CVodeFree.

F2003 Name FCVodeAdjFree

6.2.2 Forward integration function

The function CVodeF is very similar to the CVODES function CVode (see §4.5.6) in that it integrates the solution of the forward problem and returns the solution in y. At the same time, however, CVodeF stores checkpoint data every Nd integration steps. CVodeF can be called repeatedly by the user. Note that CVodeF 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

CVodeF

Call `flag = CVodeF(cvode_mem, tout, yret, &tret, itask, &ncheck);`

Description The function CVodeF integrates the forward problem over an interval in t and saves checkpointing data.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block.
tout	(realtype) the next time at which a computed solution is desired.
yret	(N_Vector) the computed solution vector y.
tret	(realtype) the time reached by the solver (output).
itask	(int) a flag indicating the job of the solver for the next step. The CV_NORMAL task is to have the solver take internal steps until it has reached or just passed the user-specified tout parameter. The solver then interpolates in order to return an approximate value of y(tout). The CV_ONE_STEP option tells the solver to just take 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, `CVodeF` returns the vector `yret` and a corresponding independent variable value $t =$ `tret`, such that `yret` is the computed value of $y(t)$. Additionally, it returns in `ncheck` the number of internal checkpoints saved; the total number of checkpoint intervals is `ncheck`+1. The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.6.

`CV_SUCCESS`	`CVodeF` succeeded.
`CV_TSTOP_RETURN`	`CVodeF` succeeded by reaching the optional stopping point.
`CV_ROOT_RETURN`	`CVodeF` succeeded and found one or more roots. In this case, `tret` is the location of the root. If `nrtfn` > 1, call `CVodeGetRootInfo` to see which g_i were found to have a root.
`CV_NO_MALLOC`	The function `CVodeInit` has not been previously called.
`CV_ILL_INPUT`	One of the inputs to `CVodeF` is illegal.
`CV_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tout`.
`CV_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`CV_ERR_FAILURE`	Error test failures occurred too many times during one internal time step or occurred with $\|h\| = h_{min}$.
`CV_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step or occurred with $\|h\| = h_{min}$.
`CV_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`CV_LSOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`CV_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CV_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 `CVodeF` failures.

At this time, `CVodeF` 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 CVODES 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, `CVodeF` 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 `CVodeF`, as this information is not captured in the checkpoint data.

F2003 Name `FCVodeF`

6.2.3 Backward problem initialization functions

The functions `CVodeCreateB` and `CVodeInitB` (or `CVodeInitBS`) must be called in the order listed. They instantiate a CVODES solver object, provide problem and solution specifications, and allocate internal memory for the backward problem.

`CVodeCreateB`

Call `flag = CVodeCreateB(cvode_mem, lmmB, &which);`

Description The function `CVodeCreateB` instantiates a CVODES solver object and specifies the solution method for the backward problem.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `lmmB` (`int`) specifies the linear multistep method and may be one of two possible values: `CV_ADAMS` or `CV_BDF`.
- `which` (`int`) contains the identifier assigned by CVODES for the newly created backward problem. Any call to `CVode*B` functions requires such an identifier.

Return value The return value `flag` (of type `int`) is one of:
- `CV_SUCCESS` The call to `CVodeCreateB` was successful.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_MEM_FAIL` A memory allocation request has failed.

F2003 Name `FCVodeCreateB`

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 `CVodeInitB` initializes the backward problem when it does not depend on the forward sensitivities. It is essentially a wrapper for `CVodeInit` with some particularization for backward integration, as described below.

`CVodeInitB`

Call `flag = CVodeInitB(cvode_mem, which, rhsB, tB0, yB0);`

Description The function `CVodeInitB` provides problem specification, allocates internal memory, and initializes the backward problem.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `rhsB` (`CVRhsFnB`) is the C function which computes fB, the right-hand side of the backward ODE problem. This function has the form `rhsB(t, y, yB, yBdot, 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.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeInitB` was successful.
- `CV_NO_MALLOC` The function `CVodeInit` has not been previously called.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
- `CV_ILL_INPUT` The parameter `which` represented an invalid identifier, or either `yB0` or `rhsB` was `NULL`.

Notes The memory allocated by `CVodeInitB` is deallocated by the function `CVodeAdjFree`.

F2003 Name `FCVodeInitB`

For the case when backward problem also depends on the forward sensitivities, user must call `CVodeInitBS` instead of `CVodeInitB`. Only the third argument of each function differs between these two functions.

`CVodeInitBS`

Call `flag = CVodeInitBS(cvode_mem, which, rhsBS, tB0, yB0);`

Description The function `CVodeInitBS` provides problem specification, allocates internal memory, and initializes the backward problem.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `rhsBS` (`CVRhsFnBS`) is the C function which computes fB, the right-hand side of the backward ODE problem. This function has the form `rhsBS(t, y, yS, yB, yBdot, 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.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeInitB` was successful.
- `CV_NO_MALLOC` The function `CVodeInit` has not been previously called.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
- `CV_ILL_INPUT` The parameter `which` represented an invalid identifier, either `yB0` or `rhsBS` was `NULL`, or sensitivities were not active during the forward integration.

Notes The memory allocated by `CVodeInitBS` is deallocated by the function `CVodeAdjFree`.

F2003 Name `FCVodeInitBS`

The function `CVodeReInitB` reinitializes CVODES for the solution of a series of backward problems, each identified by a value of the parameter `which`. `CVodeReInitB` is essentially a wrapper for `CVodeReInit`, and so all details given for `CVodeReInit` in §4.5.10 apply here. Also note that `CVodeReInitB` can be called to reinitialize the backward problem even it has been initialized with the sensitivity-dependent version `CVodeInitBS`. Before calling `CVodeReInitB` for a new backward problem, call any desired solution extraction functions `CVodeGet**` associated with the previous backward problem. The call to the `CVodeReInitB` function has the form

`CVodeReInitB`

Call `flag = CVodeReInitB(cvode_mem, which, tB0, yB0)`

Description The function `CVodeReInitB` reinitializes a CVODES backward problem.

Arguments
- `cvode_mem` (`void *`) pointer to CVODES memory block returned by `CVodeCreate`.
- `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.

Return value The return value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeReInitB` was successful.
- `CV_NO_MALLOC` The function `CVodeInit` has not been previously called.
- `CV_MEM_NULL` The `cvode_mem` memory block pointer was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_BAD_TB0` The final time `tB0` is outside the interval over which the forward problem was solved.
- `CV_ILL_INPUT` The parameter `which` represented an invalid identifier, or `yB0` was `NULL`.

F2003 Name `FCVodeReInitB`

6.2.4 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 `CVodeInitB` or `CVodeInitBS`.

`CVodeSStolerancesB`

Call `flag = CVodeSStolerancesB(cvode_mem, which, reltolB, abstolB);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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 value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeSStolerancesB` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_MALLOC` The allocation function `CVodeInit` has not been called.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_ILL_INPUT` One of the input tolerances was negative.

F2003 Name `FCVodeSStolerancesB`

`CVodeSVtolerancesB`

Call `flag = CVodeSVtolerancesB(cvode_mem, which, reltolB, abstolB);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `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 value `flag` (of type `int`) will be one of the following:
- `CV_SUCCESS` The call to `CVodeSVtolerancesB` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_MALLOC` The allocation function `CVodeInit` has not been called.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_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 `FCVodeSVtolerancesB`

6.2.5 Linear solver initialization functions for backward problem

All CVODES linear solver modules available for forward problems are available for the backward problem. They should be created as for the forward problem and then attached to the memory structure for the backward problem using the following functions.

`CVodeSetLinearSolverB`

Call `flag = CVodeSetLinearSolverB(cvode_mem, which, LS, A);`

Description The function `CVodeSetLinearSolverB` attaches a generic SUNLINSOL object `LS` and corresponding template Jacobian SUNMATRIX object `A` to CVODES, initializing the CVLS linear solver interface for solution of the backward problem.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `which` (`int`) represents the identifier of the backward problem returned by `CVodeCreateB`.
- `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

`CVLS_SUCCESS` The CVLS initialization was successful.

`CVLS_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVLS_ILL_INPUT` The CVLS solver is not compatible with the current NVECTOR module.

`CVLS_MEM_FAIL` A memory allocation request failed.

`CVLS_NO_ADJ` The function `CVAdjInit` has not been previously called.

`CVLS_ILL_INPUT` The parameter `which` represented an invalid identifier.

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 9 for further information).

The previous routines `CVDlsSetLinearSolverB` and `CVSpilsSetLinearSolverB` 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 `FCVodeSetLinearSolverB`

`CVDiagB`

Call `flag = CVDiagB(cvode_mem, which);`

Description The function `CVDiagB` selects the CVDIAG linear solver for the solution of the backward problem.

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `which` (`int`) represents the identifier of the backward problem returned by `CVodeCreateB`.

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

`CVDIAG_SUCCESS` The CVDIAG initialization was successful.

`CVDIAG_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVDIAG_ILL_INPUT` The CVDIAG solver is not compatible with the current NVECTOR module.

`CVDIAG_MEM_FAIL` A memory allocation request failed.

Notes The CVDIAG solver is the simplest of all of the available CVODES linear solver interfaces. The CVDIAG solver uses an approximate diagonal Jacobian formed by way of a difference quotient. The user does *not* have the option of supplying a function to compute an approximate diagonal Jacobian.

F2003 Name `FCVDiagB`

6.2.6 Backward integration function

The function `CVodeB` performs the integration of the backward problem. It is essentially a wrapper for the CVODES main integration function `CVode` 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. The first run of each pair 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 `CVodeB` does not return the solution `yB` itself. To obtain that, call the function `CVodeGetB`, which is also described below.

The `CVodeB` function does not support rootfinding, unlike `CVodeF`, which supports the finding of roots of functions of (t, y). If rootfinding was performed by `CVodeF`, then for the sake of efficiency, it should be disabled for `CVodeB` by first calling `CVodeRootInit` with `nrtfn` $= 0$.

The call to `CVodeB` has the form

`CVodeB`

Call `flag = CVodeB(cvode_mem, tBout, itaskB);`

Description The function `CVodeB` integrates the backward ODE problem.

Arguments

`cvode_mem`	(`void *`) pointer to the CVODES memory returned by `CVodeCreate`.
`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 `CV_NORMAL` task is to have the solver take internal steps until it has reached or just passed the user-specified value `tBout`. The solver then interpolates in order to return an approximate value of yB(`tBout`). The `CV_ONE_STEP` option tells the solver to take just one internal step in the direction of `tBout` and return.

Return value The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.6.

`CV_SUCCESS`	`CVodeB` succeeded.
`CV_MEM_NULL`	`cvode_mem` was `NULL`.
`CV_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CV_NO_BCK`	No backward problem has been added to the list of backward problems by a call to `CVodeCreateB`
`CV_NO_FWD`	The function `CVodeF` has not been previously called.
`CV_ILL_INPUT`	One of the inputs to `CVodeB` is illegal.
`CV_BAD_ITASK`	The `itaskB` argument has an illegal value.
`CV_TOO_MUCH_WORK`	The solver took `mxstep` internal steps but could not reach `tBout`.
`CV_TOO_MUCH_ACC`	The solver could not satisfy the accuracy demanded by the user for some internal step.
`CV_ERR_FAILURE`	Error test failures occurred too many times during one internal time step.
`CV_CONV_FAILURE`	Convergence test failures occurred too many times during one internal time step.
`CV_LSETUP_FAIL`	The linear solver's setup function failed in an unrecoverable manner.
`CV_SOLVE_FAIL`	The linear solver's solve function failed in an unrecoverable manner.
`CV_BCKMEM_NULL`	The solver memory for the backward problem was not created with a call to `CVodeCreateB`.

CV_BAD_TBOUT	The desired output time tBout is outside the interval over which the forward problem was solved.
CV_REIFWD_FAIL	Reinitialization of the forward problem failed at the first checkpoint (corresponding to the initial time of the forward problem).
CV_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 CVodeB failures.

In the case of multiple checkpoints and multiple backward problems, a given call to CVodeB in CV_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 FCVodeB

To obtain the solution yB to the backward problem, call the function CVodeGetB as follows:

CVodeGetB

Call `flag = CVodeGetB(cvode_mem, which, &tret, yB);`

Description The function CVodeGetB provides the solution yB of the backward ODE problem.

Arguments

cvode_mem	(void *) pointer to the CVODES memory returned by CVodeCreate.
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.

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

CV_SUCCESS	CVodeGetB was successful.
CV_MEM_NULL	cvode_mem is NULL.
CV_NO_ADJ	The function CVodeAdjInit has not been previously called.
CV_ILL_INPUT	The parameter which is an invalid identifier.

Notes The user must allocate space for yB.

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 CVODES memory structure by calling CVodeGetAdjCVodeBmem and then use it to call CVodeGetDky.

F2003 Name FCVodeGetB

6.2.7 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:

CVodeAdjSetNoSensi

Call `flag = CVodeAdjSetNoSensi(cvode_mem);`

Description The function CVodeAdjSetNoSensi instructs CVodeF not to save checkpointing data for forward sensitivities anymore.

Arguments cvode_mem (void *) pointer to the CVODES memory block.

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

CV_SUCCESS	The call to CVodeCreateB was successful.
CV_MEM_NULL	cvode_mem was NULL.
CV_NO_ADJ	The function CVodeAdjInit has not been previously called.

F2003 Name FCVodeAdjSetNoSensi

6.2.8 Optional input functions for the backward problem

6.2.8.1 Main solver optional input functions

The adjoint module in CVODES provides wrappers for most of the optional input functions defined in §4.5.7.1. The only difference is that the user must specify the identifier `which` of the backward problem within the list managed by CVODES.

The optional input functions defined for the backward problem are:

```
flag = CVodeSetNonlinearSolverB(cvode_mem, which, NLSB);
flag = CVodeSetUserDataB(cvode_mem, which, user_dataB);
flag = CVodeSetMaxOrdB(cvode_mem, which, maxordB);
flag = CVodeSetMaxNumStepsB(cvode_mem, which, mxstepsB);
flag = CVodeSetInitStepB(cvode_mem, which, hinB)
flag = CVodeSetMinStepB(cvode_mem, which, hminB);
flag = CVodeSetMaxStepB(cvode_mem, which, hmaxB);
flag = CVodeSetStabLimDetB(cvode_mem, which, stldetB);
flag = CVodeSetConstraintsB(cvode_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 `CV_NO_ADJ` if `CVodeAdjInit` has not been called, or `CV_ILL_INPUT` if `which` was an invalid identifier.

6.2.8.2 Linear solver interface optional input functions

When using matrix-based linear solver modules, the CVLS solver interface needs a function to compute an approximation to the Jacobian matrix or the linear system for the backward problem. The function to evaluate the Jacobian can be attached through a call to either `CVodeSetJacFnB` or `CVodeSetJacFnBS`, with the second used when the backward problem depends on the forward sensitivities.

`CVodeSetJacFnB`

Call `flag = CVodeSetJacFnB(cvode_mem, which, jacB);`

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

Arguments

`cvode_mem`	(`void *`)	pointer to the CVODES memory returned by `CVodeCreate`.
`which`	(`int`)	represents the identifier of the backward problem.
`jacB`	(`CVLsJacFnB`)	user-defined Jacobian approximation function.

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

`CVLS_SUCCESS`	`CVodeSetJacFnB` succeeded.
`CVLS_MEM_NULL`	`cvode_mem` was `NULL`.
`CVLS_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CVLS_LMEM_NULL`	The linear solver has not been initialized with a call to `CVodeSetLinearSolverB`.
`CVLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `CVLsJacFnB` is described in §6.3.5.

The previous routine `CVDlsSetJacFnB` 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 `FCVodeSetJacFnB`

`CVodeSetJacFnBS`

Call `flag = CVodeSetJacFnBS(cvode_mem, which, jacBS);`

Description The function `CVodeSetJacFnBS` 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
`cvode_mem` (`void *`) pointer to the CVODES memory returned by `CVodeCreate`.
`which` (`int`) represents the identifier of the backward problem.
`jacBS` (`CVLsJacFnBS`) user-defined Jacobian approximation function.

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

`CVLS_SUCCESS`	`CVodeSetJacFnBS` succeeded.
`CVLS_MEM_NULL`	`cvode_mem` was `NULL`.
`CVLS_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CVLS_LMEM_NULL`	The linear solver has not been initialized with a call to `CVodeSetLinearSolverB`.
`CVLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `CVLsJacFnBS` is described in §6.3.5.

The previous routine `CVDlsSetJacFnBS` 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 `FCVodeSetJacFnBS`

Alternatively, a function to evaluate the linear system can be attached through a call to either `CVodeSetLinSysFnB` or `CVodeSetLinSysFnBS`, with the second used when the backward problem depends on the forwrad sensitivities.

`CVodeSetLinSysFnB`

Call `flag = CVodeSetLinSysFnB(cvode_mem, which, linsysB);`

Description The function `CVodeSetLinSysFnB` specifies the linear system approximation function to be used for the backward problem.

Arguments
`cvode_mem` (`void *`) pointer to the CVODES memory returned by `CVodeCreate`.
`which` (`int`) represents the identifier of the backward problem.
`linsysB` (`CVLsLinSysFnB`) user-defined linear system approximation function.

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

`CVLS_SUCCESS`	`CVodeSetLinSysFnB` succeeded.
`CVLS_MEM_NULL`	`cvode_mem` was `NULL`.
`CVLS_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CVLS_LMEM_NULL`	The linear solver has not been initialized with a call to `CVodeSetLinearSolverB`.
`CVLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `CVLsLinSysFnB` is described in §**??**.

F2003 Name `FCVodeSetLinSysFnB`

`CVodeSetLinSysFnBS`

Call `flag = CVodeSetLinSysFnBS(cvode_mem, which, linsysBS);`

Description The function `CVodeSetLinSysFnBS` specifies the linear system approximation function to be used for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory returned by `CVodeCreate`.
`which` (`int`) represents the identifier of the backward problem.
`linsysBS` (`CVLsLinSysFnBS`) user-defined linear system approximation function.

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

`CVLS_SUCCESS`	`CVodeSetLinSysFnBS` succeeded.
`CVLS_MEM_NULL`	`cvode_mem` was `NULL`.
`CVLS_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CVLS_LMEM_NULL`	The linear solver has not been initialized with a call to `CVodeSetLinearSolverB`.
`CVLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function type `CVLsLinSysFnBS` is described in §**??**.

F2003 Name `FCVodeSetLinSysFnBS`

`CVodeSetJacTimesB`

Call `flag = CVodeSetJacTimesB(cvode_mem, which, jsetupB, jtvB);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`which` (`int`) the identifier of the backward problem.
`jtsetupB` (`CVLsJacTimesSetupFnB`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.
`jtvB` (`CVLsJacTimesVecFnB`) user-defined Jacobian-vector product function.

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

`CVLS_SUCCESS`	The optional value has been successfully set.
`CVLS_MEM_NULL`	`cvode_mem` was `NULL`.
`CVLS_LMEM_NULL`	The CVLS linear solver has not been initialized.
`CVLS_NO_ADJ`	The function `CVodeAdjInit` has not been previously called.
`CVLS_ILL_INPUT`	The parameter `which` represented an invalid identifier.

Notes The function types `CVLsJacTimesVecFnB` and `CVLsJacTimesSetupFnB` are described in §6.3.7.

The previous routine `CVSpilsSetJacTimesB` 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 `FCVodeSetJacTimesB`

`CVodeSetJacTimesBS`

Call `flag = CVodeSetJacTimesBS(cvode_mem, which, jtvBS);`

Description The function `CVodeSetJacTimesBS` specifies the Jacobian-vector setup and product functions to be used, in the case where the backward problem depends on the forward sensitivities.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.
`which` (`int`) the identifier of the backward problem.
`jtsetupBS` (`CVLsJacTimesSetupFnBS`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.
`jtvBS` (`CVLsJacTimesVecFnBS`) user-defined Jacobian-vector product function.

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

CVLS_SUCCESS	The optional value has been successfully set.
CVLS_MEM_NULL	cvode_mem was NULL.
CVLS_LMEM_NULL	The CVLS linear solver has not been initialized.
CVLS_NO_ADJ	The function CVodeAdjInit has not been previously called.
CVLS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function types CVLsJacTimesVecFnBS and CVLsJacTimesSetupFnBS are described in §6.3.7.

The previous routine CVSpilsSetJacTimesBS 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 FCVodeSetJacTimesBS

CVodeSetPreconditionerB

Call `flag = CVodeSetPreconditionerB(cvode_mem, which, psetupB, psolveB);`

Description The function CVodeSetPrecSolveFnB specifies the preconditioner setup and solve functions for the backward integration.

Arguments
cvode_mem (void *) pointer to the CVODES memory block.
which (int) the identifier of the backward problem.
psetupB (CVLPrecSetupFnB) user-defined preconditioner setup function.
psolveB (CVLsPrecSolveFnB) user-defined preconditioner solve function.

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

CVLS_SUCCESS	The optional value has been successfully set.
CVLS_MEM_NULL	cvode_mem was NULL.
CVLS_LMEM_NULL	The CVLS linear solver has not been initialized.
CVLS_NO_ADJ	The function CVodeAdjInit has not been previously called.
CVLS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function types CVLsPrecSolveFnB and CVLsPrecSetupFnB are described in §6.3.9 and §6.3.10, respectively. The psetupB argument may be NULL if no setup operation is involved in the preconditioner.

The previous routine CVSpilsSetPrecSolveFnB 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 FCVodeSetPreconditionerB

CVodeSetPreconditionerBS

Call `flag = CVodeSetPreconditionerBS(cvode_mem, which, psetupBS, psolveBS);`

Description The function CVodeSetPrecSolveFnBS specifies the preconditioner setup and solve functions for the backward integration, in the case where the backward problem depends on the forward sensitivities.

Arguments
cvode_mem (void *) pointer to the CVODES memory block.
which (int) the identifier of the backward problem.
psetupBS (CVLsPrecSetupFnBS) user-defined preconditioner setup function.
psolveBS (CVLsPrecSolveFnBS) user-defined preconditioner solve function.

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

CVLS_SUCCESS	The optional value has been successfully set.
CVLS_MEM_NULL	cvode_mem was NULL.

CVLS_LMEM_NULL	The CVLS linear solver has not been initialized.
CVLS_NO_ADJ	The function CVodeAdjInit has not been previously called.
CVLS_ILL_INPUT	The parameter which represented an invalid identifier.

Notes The function types CVodePrecSolveFnBS and CVodePrecSetupFnBS are described in §6.3.9 and §6.3.10, respectively. The psetupBS argument may be NULL if no setup operation is involved in the preconditioner.

The previous routine CVSpilsSetPrecSolveFnBS 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 FCVodeSetPreconditionerBS

CVodeSetEpsLinB

Call `flag = CVodeSetEpsLinB(cvode_mem, which, eplifacB);`

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

Arguments
cvode_mem	(void *) pointer to the CVODES memory block.
which	(int) the identifier of the backward problem.
eplifacB	(realtype) value of the convergence test constant reduction factor (≥ 0.0).

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

CVLS_SUCCESS	The optional value has been successfully set.
CVLS_MEM_NULL	cvode_mem was NULL.
CVLS_LMEM_NULL	The CVLS linear solver has not been initialized.
CVLS_NO_ADJ	The function CVodeAdjInit has not been previously called.
CVLS_ILL_INPUT	The parameter which represented an invalid identifier, or eplifacB was negative.

Notes The default value is 0.05. Passing a value eplifacB$= 0.0$ also indicates using the default value.

The previous routine CVSpilsSetEpsLinB 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 FCVodeSetEpsLinB

6.2.9 Optional output functions for the backward problem

The user of the adjoint module in CVODES has access to any of the optional output functions described in §4.5.9, both for the main solver and for the linear solver modules. The first argument of these CVodeGet* and CVode*Get* functions is the pointer to the CVODES 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.

CVodeGetAdjCVodeBmem

Call `cvode_memB = CVodeGetAdjCVodeBmem(cvode_mem, which);`

Description The function CVodeGetAdjCVodeBmem returns a pointer to the CVODES memory block for the backward problem.

Arguments cvode_mem (void *) pointer to the CVODES memory block created by CVodeCreate.

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

Return value The return value, `cvode_memB` (of type `void *`), is a pointer to the CVODES memory for the backward problem.

Notes The user should not modify `cvode_memB` in any way.

Optional output calls should pass `cvode_memB` as the first argument; for example, to get the number of integration steps: `flag = CVodeGetNumSteps(cvodes_memB, &nsteps)`.

F2003 Name `FCVodeGetAdjCVodeBmem`

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 `CVodeGetB`. In any case, it must be within the last checkpoint interval used by `CVodeB`.

`CVodeGetAdjY`

Call `flag = CVodeGetAdjY(cvode_mem, t, y);`

Description The function `CVodeGetAdjY` returns the interpolated value of the forward solution y during a backward integration.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block created by `CVodeCreate`.

`t` (`realtype`) value of the independent variable at which y is desired (input).

`y` (`N_Vector`) forward solution $y(t)$.

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

`CV_SUCCESS` `CVodeGetAdjY` was successful.

`CV_MEM_NULL` `cvode_mem` was `NULL`.

`CV_GETY_BADT` The value of `t` was outside the current checkpoint interval.

Notes The user must allocate space for `y`.

F2003 Name `FCVodeGetAdjY`

`CVodeGetAdjCheckPointsInfo`

Call `flag = CVodeGetAdjCheckPointsInfo(cvode_mem, CVadjCheckPointRec *ckpnt);`

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block created by `CVodeCreate`.

`ckpnt` (`CVadjCheckPointRec *`) array of `ncheck+1` checkpoint records, each of type `CVadjCheckPointRec`.

Return value The return value is `CV_SUCCESS` if successful, or `CV_MEM_NULL` if `cvode_mem` is `NULL`, or `CV_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 `cvode_mem->cv_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 `FCVodeGetAdjCheckPointsInfo`

6.2.10 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, either `CVodeQuadInitB` or `CVodeQuadInitBS` 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 callable regardless of whether or not the quadratures are sensitivity-dependent.

6.2.10.1 Backward quadrature initialization functions

The function `CVodeQuadInitB` initializes and allocates memory for the backward integration of quadrature equations that do not depend on forward sensitivities. It has the following form:

`CVodeQuadInitB`

Call `flag = CVodeQuadInitB(cvode_mem, which, rhsQB, yQB0);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `which` (`int`) the identifier of the backward problem.
- `rhsQB` (`CVQuadRhsFnB`) is the C function which computes fQB, the right-hand side of the backward quadrature equations. This function has the form `rhsQB(t, y, yB, qBdot, 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:
- `CV_SUCCESS` The call to `CVodeQuadInitB` was successful.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_MEM_FAIL` A memory allocation request has failed.
- `CV_ILL_INPUT` The parameter `which` is an invalid identifier.

F2003 Name `FCVodeQuadInitB`

The function `CVodeQuadInitBS` initializes and allocates memory for the backward integration of quadrature equations that depends on the forward sensitivities.

`CVodeQuadInitBS`

Call `flag = CVodeQuadInitBS(cvode_mem, which, rhsQBS, yQBS0);`

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

Arguments
- `cvode_mem` (`void *`) pointer to the CVODES memory block.
- `which` (`int`) the identifier of the backward problem.
- `rhsQBS` (`CVQuadRhsFnBS`) is the C function which computes $fQBS$, the right-hand side of the backward quadrature equations. This function has the form `rhsQBS(t, y, yS, yB, qBdot, 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:
- `CV_SUCCESS` The call to `CVodeQuadInitBS` was successful.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_MEM_FAIL` A memory allocation request has failed.

CV_ILL_INPUT The parameter which is an invalid identifier.

F2003 Name FCVodeQuadInitBS

The integration of quadrature equations during the backward phase can be re-initialized by calling the following function. Before calling CVodeQuadReInitB for a new backward problem, call any desired solution extraction functions CVodeGet** associated with the previous backward problem.

CVodeQuadReInitB

Call `flag = CVodeQuadReInitB(cvode_mem, which, yQB0);`

Description The function CVodeQuadReInitB re-initializes the backward quadrature integration.

Arguments
- cvode_mem (void *) pointer to the CVODES 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:
- CV_SUCCESS The call to CVodeQuadReInitB was successful.
- CV_MEM_NULL cvode_mem was NULL.
- CV_NO_ADJ The function CVodeAdjInit has not been previously called.
- CV_MEM_FAIL A memory allocation request has failed.
- CV_NO_QUAD Quadrature integration was not activated through a previous call to CVodeQuadInitB.
- CV_ILL_INPUT The parameter which is an invalid identifier.

Notes The function CVodeQuadReInitB can be called after a call to either CVodeQuadInitB or CVodeQuadInitBS.

F2003 Name FCVodeQuadReInitB

6.2.10.2 Backward quadrature extraction function

To extract the values of the quadrature variables at the last return time of CVodeB, CVODES provides a wrapper for the function CVodeGetQuad (see §4.7.3). The call to this function has the form

CVodeGetQuadB

Call `flag = CVodeGetQuadB(cvode_mem, which, &tret, yQB);`

Description The function CVodeGetQuadB returns the quadrature solution vector after a successful return from CVodeB.

Arguments
- cvode_mem (void *) pointer to the CVODES memory.
- tret (realtype) the time reached by the solver (output).
- yQB (N_Vector) the computed quadrature vector.

Return value The return value flag of CVodeGetQuadB is one of:
- CV_SUCCESS CVodeGetQuadB was successful.
- CV_MEM_NULL cvode_mem is NULL.
- CV_NO_ADJ The function CVodeAdjInit has not been previously called.
- CV_NO_QUAD Quadrature integration was not initialized.
- CV_BAD_DKY yQB was NULL.
- CV_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 CVODES memory structure by calling CVodeGetAdjCVodeBmem and then use it to call CVodeGetQuadDky.

F2003 Name FCVodeGetQuadB

6.2.10.3 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 = CVodeSetQuadErrConB(cvode_mem, which, errconQ);
flag = CVodeQuadSStolerancesB(cvode_mem, which, reltolQ, abstolQ);
flag = CVodeQuadSVtolerancesB(cvode_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 `CV_NO_ADJ` if the function `CVodeAdjInit` has not been previously called or `CV_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 `CVodeGetQuad*` functions (see §4.7.5). A pointer `cvode_memB` to the CVODES memory block for the backward problem, required as the first argument of these functions, can be obtained through a call to the functions `CVodeGetAdjCVodeBmem` (see §6.2.9).

6.3 User-supplied functions for adjoint sensitivity analysis

In addition to the required ODE right-hand side function and any optional functions for the forward problem, when using the adjoint sensitivity module in CVODES, the user must supply one function defining the backward problem ODE and, optionally, functions to supply Jacobian-related information and one or two functions that define the preconditioner (if an iterative SUNLINSOL module is selected) for the backward problem. Type definitions for all these user-supplied functions are given below.

6.3.1 ODE right-hand side for the backward problem

If the backward problem does not depend on the forward sensitivities, the user must provide a `rhsB` function of type `CVRhsFnB` defined as follows:

`CVRhsFnB`

Definition
```
typedef int (*CVRhsFnB)(realtype t, N_Vector y,
                        N_Vector yB, N_Vector yBdot, void *user_dataB);
```

Purpose This function evaluates the right-hand side $f_B(t, y, y_B)$ of the backward problem ODE system. This could be either (2.20) or (2.23).

Arguments

`t`	is the current value of the independent variable.
`y`	is the current value of the forward solution vector.
`yB`	is the current value of the backward dependent variable vector.
`yBdot`	is the output vector containing the right-hand side f_B of the backward ODE problem.
`user_dataB`	is a pointer to user data, same as passed to `CVodeSetUserDataB`.

Return value A `CVRhsFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_RHSFUNC_FAIL`).

Notes Allocation of memory for `yBdot` is handled within CVODES.

The `y`, `yB`, and `yBdot` arguments are all of type `N_Vector`, but `yB` and `yBdot` typically have different internal representations from `y`. 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 CVODES do not perform any consistency checks with respect to their N_Vector arguments (see §8.3 and §8.4).

The user_dataB pointer is passed to the user's rhsB 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 rhsB function, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the right-hand side function which will halt the integration and CVodeB will return CV_RHSFUNC_FAIL.

6.3.2 ODE right-hand side for the backward problem depending on the forward sensitivities

If the backward problem does depend on the forward sensitivities, the user must provide a rhsBS function of type CVRhsFnBS defined as follows:

CVRhsFnBS

Definition
```
typedef int (*CVRhsFnBS)(realtype t, N_Vector y, N_Vector *yS,
                         N_Vector yB, N_Vector yBdot, void *user_dataB);
```

Purpose This function evaluates the right-hand side $f_B(t, y, y_B, s)$ of the backward problem ODE system. This could be either (2.20) or (2.23).

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
yB	is the current value of the backward dependent variable vector.
yBdot	is the output vector containing the right-hand side f_B of the backward ODE problem.
user_dataB	is a pointer to user data, same as passed to CVodeSetUserDataB.

Return value A CVRhsFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and CVodeB returns CV_RHSFUNC_FAIL).

Notes Allocation of memory for qBdot is handled within CVODES.

The y, yB, and yBdot arguments are all of type N_Vector, but yB and yBdot typically have different internal representations from y. Likewise for each yS[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 CVODES do not perform any consistency checks with respect to their N_Vector arguments (see §8.3 and §8.4).

The user_dataB pointer is passed to the user's rhsBS 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 rhsBS function, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the right-hand side function which will halt the integration and CVodeB will return CV_RHSFUNC_FAIL.

6.3.3 Quadrature right-hand side for the backward problem

The user must provide an fQB function of type CVQuadRhsFnB defined by

CVQuadRhsFnB

Definition
```
typedef int (*CVQuadRhsFnB)(realtype t, N_Vector y, N_Vector yB,
                            N_Vector qBdot, 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.
- `yB` is the current value of the backward dependent variable vector.
- `qBdot` is the output vector containing the right-hand side `fQB` of the backward quadrature equations.
- `user_dataB` is a pointer to user data, same as passed to `CVodeSetUserDataB`.

Return value A `CVQuadRhsFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_QRHSFUNC_FAIL`).

Notes Allocation of memory for `rhsvalBQ` is handled within CVODES.

The `y`, `yB`, and `qBdot` arguments are all of type `N_Vector`, but they typically do not all have the same representation. 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 CVODES do not perform any consistency checks with repsect to their `N_Vector` arguments (see §8.3 and §8.4).

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, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and `CVodeB` will return `CV_QRHSFUNC_FAIL`.

6.3.4 Sensitivity-dependent quadrature right-hand side for the backward problem

The user must provide an `fQBS` function of type `CVQuadRhsFnBS` defined by

CVQuadRhsFnBS

Definition
```
typedef int (*CVQuadRhsFnBS)(realtype t, N_Vector y, N_Vector *yS,
                             N_Vector yB, N_Vector qBdot,
                             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.
- `yS` a pointer to an array of `Ns` vectors containing the sensitivities of the forward solution.
- `yB` is the current value of the backward dependent variable vector.
- `qBdot` is the output vector containing the right-hand side `fQBS` of the backward quadrature equations.
- `user_dataB` is a pointer to user data, same as passed to `CVodeSetUserDataB`.

Return value A CVQuadRhsFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and CVodeB returns CV_QRHSFUNC_FAIL).

Notes Allocation of memory for qBdot is handled within CVODES.

The y, yS, and qBdot arguments are all of type N_Vector, but they typically do not all have the same internal representation. Likewise for each yS[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 CVODES do not perform any consistency checks with repsect to their N_Vector arguments (see §8.3 and §8.4).

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, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and CVodeB will return CV_QRHSFUNC_FAIL.

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

If a matrix-based linear solver module is used for the backward problem (i.e., a non-NULL SUNMATRIX object was supplied to CVodeSetLinearSolverB), the user may provide a function of type CVLsJacFnB or CVLsJacFnBS (see §6.2.8), defined as follows:

CVLsJacFnB

Definition
```
typedef int (*CVLsJacFnB)(realtype t, N_Vector y,
                          N_Vector yB, N_Vector fyB,
                          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

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
JacB	is the output approximate Jacobian matrix.
user_dataB	is a pointer to user data – the same as passed to CVodeSetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by the CVLsJacFnB function as temporary storage or work space.

Return value A CVLsJacFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct, while CVLS sets last_flag to CVLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

Notes A user-supplied Jacobian function must load the matrix JacB with an approximation to the Jacobian matrix at the point (t,y,yB), where y 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 9 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 CVLsJacFnB, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the Jacobian function which will halt the integration (CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

The previous function type CVDlsJacFnB is identical to CVLsJacFnB, 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.

CVLsJacFnBS

Definition
```
typedef int (*CVLsJacFnBS)(realtype t, N_Vector y,
                           N_Vector *yS, N_Vector yB, N_Vector fyB,
                           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

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
JacB	is the output approximate Jacobian matrix.
user_dataB	is a pointer to user data – the same as passed to CVodeSetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by CVLsJacFnBS as temporary storage or work space.

Return value A CVLsJacFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct, while CVLS sets last_flag to CVLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

Notes A user-supplied Jacobian function must load the matrix JacB with an approximation to the Jacobian matrix at the point (t,y,yS,yB), where y is the solution of the original IVP at time tt, yS is the vector 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 9 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 CVLsJacFnBS, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the Jacobian function which will halt the integration (CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

The previous function type CVDlsJacFnBS is identical to CVLsJacFnBS, 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 Linear system construction for the backward problem (matrix-based linear solvers)

With matrix-based linear solver modules, as an alternative to optionally supplying a function for evaluating the Jacobian of the ODE right-hand side function, the user may optionally supply a function of type CVLsLinSysFnB or CVLsLinSysFnBS (see §6.2.8) for evaluating the linear system, $M_B = I - \gamma_B J_B$ (or an approximation of it) for the backward problem.

CVLsLinSysFnB

Definition
```
typedef int (*CVLsLinSysFnB)(realtype t, N_Vector y, N_Vector yB,
                             N_Vector fyB, SUNMatrix AB,
                             booleantype jokB, booleantype *jcurB,
                             realtype gammaB, void *user_dataB,
                             N_Vector tmp1B, N_Vector tmp2B,
                             N_Vector tmp3B);
```

Purpose This function computes the linear system of the backward problem (or an approximation to it).

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
MB	is the output approximate linear system matrix.
jokB	is an input flag indicating whether Jacobian-related data needs to be recomputed (jokB=SUNFALSE) or information saved from a previous invokation can be safely used (jokB=SUNTRUE).
jcurB	is an output flag which must be set to SUNTRUE if Jacobian-relatd data was recomputed or SUNFALSE otherwise.
gammaB	is the scalar appearing in the matrix $M_B = I - \gamma_B J_B$.
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to CVodeSetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by the CVLsLinSysFnB function as temporary storage or work space.

Return value A CVLsLinSysFnB should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct, while CVLS sets last_flag to CVLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case

the integration is halted, CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

Notes A user-supplied linear system function must load the matrix MB with an approximation to the linear system matrix at the point (t, y, yB), where y is the solution of the original IVP at time tt, and yB is the solution of the backward problem at the same time.

Before calling the user's CVLsLinSysFnB, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the linear system function which will halt the integration (CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

CVLsLinSysFnBS

Definition
```
typedef int (*CVLsLinSysFnBS)(realtype t, N_Vector y, N_Vector* yS,
                              N_Vector yB, N_Vector fyB, SUNMatrix MB,
                              booleantype jokB, booleantype *jcurB,
                              realtype gammaB, void *user_dataB,
                              N_Vector tmp1B, N_Vector tmp2B,
                              N_Vector tmp3B);
```

Purpose This function computes the linear system of the backward problem (or an approximation to it), in the case where the backward problem depends on the forward sensitivities.

Arguments

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yS	a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
MB	is the output approximate linear system matrix.
jokB	is an input flag indicating whether Jacobian-related data needs to be recomputed (jokB=SUNFALSE) or information saved from a previous invokation can be safely used (jokB=SUNTRUE).
jcurB	is an output flag which must be set to SUNTRUE if Jacobian-relatd data was recomputed or SUNFALSE otherwise.
gammaB	is the scalar appearing in the matrix $M_B = I - \gamma_B J_B$.
user_dataB	is a pointer to user data – the same as passed to CVodeSetUserDataB.
tmp1B	
tmp2B	
tmp3B	are pointers to memory allocated for variables of type N_Vector which can be used by CVLsLinSysFnBS as temporary storage or work space.

Return value A CVLsLinSysFnBS should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct, while CVLS sets last_flag to CVLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

Notes A user-supplied linear system function must load the matrix MB with an approximation to the linear system matrix at the point (t, y, yS, yB), where y is the solution of the original IVP at time tt, yS is the vector of forward sensitivities at time t, and yB is the solution of the backward problem at the same time.

Before calling the user's CVLsLinSysFnBS, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in

the interpolation, CVODES triggers an unrecoverable failure in the linear system function which will halt the integration (CVodeB returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

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

If a matrix-free linear solver is to be used for the backward problem (i.e., a NULL-valued SUNMATRIX was supplied to CVodeSetLinearSolverB in the steps described in §6.1), the user may provide a function of type CVLsJacTimesVecFnB or CVLsJacTimesVecFnBS 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.

CVLsJacTimesVecFnB

Definition
```
typedef int (*CVLsJacTimesVecFnB)(N_Vector vB, N_Vector JvB,
                                  realtype t, N_Vector y, N_Vector yB,
                                  N_Vector fyB, void *user_dataB,
                                  N_Vector tmpB);
```

Purpose This function computes the action of the Jacobian JB for the backward problem on a given vector vB.

Arguments

vB	is the vector by which the Jacobian must be multiplied to the right.
JvB	is the computed output vector JB*vB.
t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
user_dataB	is a pointer to user data – the same as passed to CVodeSetUserDataB.
tmpB	is a pointer to memory allocated for a variable of type N_Vector which can be used by CVLsJacTimesVecFn as temporary storage or work space.

Return value The return value of a function of type CVLsJacTimesVecFnB 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 CVLsJacTimesVecFn (see §4.6.7). 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 CVSpilsJacTimesVecFnB is identical to CVLsJacTimesVecFnB, 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.

CVLsJacTimesVecFnBS

Definition
```
typedef int (*CVLsJacTimesVecFnBS)(N_Vector vB, N_Vector JvB,
                                   realtype t, N_Vector y, N_Vector *yS,
                                   N_Vector yB, N_Vector fyB,
                                   void *user_dataB, N_Vector tmpB);
```

Purpose This function computes the action of the Jacobian JB for the backward problem on a given vector vB, in the case where the backward problem depends on the forward sensitivities.

Arguments
- `vB` is the vector by which the Jacobian must be multiplied to the right.
- `JvB` is the computed output vector `JB*vB`.
- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yS` is a pointer to an array containing the forward sensitivity vectors.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function f_B.
- `user_dataB` is a pointer to user data – the same as passed to `CVodeSetUserDataB`.
- `tmpB` is a pointer to memory allocated for a variable of type `N_Vector` which can be used by `CVLsJacTimesVecFn` as temporary storage or work space.

Return value The return value of a function of type `CVLsJacTimesVecFnBS` 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 `CVLsJacTimesVecFn` (see §4.6.7).

The previous function type `CVSpilsJacTimesVecFnBS` is identical to `CVLsJacTimesVecFnBS`, 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 Jacobian-vector product setup for the backward problem (matrix-free linear solvers)

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

`CVLsJacTimesSetupFnB`

Definition
```
typedef int (*CVLsJacTimesSetupFnB)(realtype t,
                                    N_Vector y, N_Vector yB,
                                    N_Vector fyB, void *user_dataB);
```

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

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector, $y(t)$.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the right-hand-side for the backward problem.
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVSetUserDataB`.

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, yB)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the right-hand-side function.

If the user's CVLsJacTimesVecFnB 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 cvode_mem to user_dataB and then use the CVGet* functions described in §4.5.9.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

The previous function type CVSpilsJacTimesSetupFnB is identical to CVLsJacTimesSetupFnB, 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.

CVLsJacTimesSetupFnBS

Definition
```
typedef int (*CVLsJacTimesSetupFnBS)(realtype t,
                                     N_Vector y, N_Vector *yS,
                                     N_Vector yB, N_Vector fyB,
                                     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
- t — is the current value of the independent variable.
- y — is the current value of the dependent variable vector, $y(t)$.
- yS — a pointer to an array of Ns vectors containing the sensitivities of the forward solution.
- yB — is the current value of the backward dependent variable vector.
- fyB — is the current value of the right-hand-side function for the backward problem.
- user_dataB — is a pointer to user data — the same as the user_dataB parameter passed to CVSetUserDataB.

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, yS, yB) arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the right-hand-side function.

If the user's CVLsJacTimesVecFnBS 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 cvode_mem to user_dataB and then use the CVGet* functions described in §4.5.9.2. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

The previous function type CVSpilsJacTimesSetupFnBS is identical to CVLsJacTimesSetupFnBS, 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 solve for the backward problem (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 may be either a left or a right preconditioner matrix. Here P should approximate (at least crudely) the matrix $M_B = I - \gamma_B J_B$, where $J_B = \partial f_B / \partial y_B$. If preconditioning is done on both sides, the product of the two preconditioner matrices should approximate M_B. This function must be of one of the following two types:

CVLsPrecSolveFnB

Definition
```
typedef int (*CVLsPrecSolveFnB)(realtype t, N_Vector y,
                                N_Vector yB, N_Vector fyB,
                                N_Vector rvecB, N_Vector zvecB,
                                realtype gammaB, realtype deltaB,
                                void *user_dataB);
```

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

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function f_B.
- `rvecB` is the right-hand side vector r of the linear system to be solved.
- `zvecB` is the computed output vector.
- `gammaB` is the scalar appearing in the matrix, $M_B = I - \gamma_B J_B$.
- `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 `CVodeSetUserDataB`.

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 `CVSpilsPrecSolveFnB` is identical to `CVLsPrecSolveFnB`, 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.

CVLsPrecSolveFnBS

Definition
```
typedef int (*CVLsPrecSolveFnBS)(realtype t, N_Vector y, N_Vector *yS,
                                 N_Vector yB, N_Vector fyB,
                                 N_Vector rvecB, N_Vector zvecB,
                                 realtype gammaB, realtype deltaB,
                                 void *user_dataB);
```

Purpose This function solves the preconditioning system $Pz = r$ for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments
- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yS` is a pointer to an array containing the forward sensitivity vectors.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function f_B.
- `rvecB` is the right-hand side vector r of the linear system to be solved.
- `zvecB` is the computed output vector.
- `gammaB` is the scalar appearing in the matrix, $M_B = I - \gamma_B J_B$.
- `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 `CVodeSetUserDataB`.

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 CVSpilsPrecSolveFnBS is identical to CVLsPrecSolveFnBS, 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.

6.3.10 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:

CVLsPrecSetupFnB

Definition
```
typedef int (*CVLsPrecSetupFnB)(realtype t, N_Vector y,
                                N_Vector yB, N_Vector fyB,
                                booleantype jokB, booleantype *jcurPtrB,
                                realtype gammaB, 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 a CVLsPrecSetupFnB are as follows:

t	is the current value of the independent variable.
y	is the current value of the forward solution vector.
yB	is the current value of the backward dependent variable vector.
fyB	is the current value of the backward right-hand side function f_B.
jokB	is an input flag indicating whether Jacobian-related data needs to be recomputed (jokB=SUNFALSE) or information saved from a previous invokation can be safely used (jokB=SUNTRUE).
jcurPtr	is an output flag which must be set to SUNTRUE if Jacobian-relatd data was recomputed or SUNFALSE otherwise.
gammaB	is the scalar appearing in the matrix $M_B = I - \gamma_B J_B$.
user_dataB	is a pointer to user data — the same as the user_dataB parameter passed to CVodeSetUserDataB.

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 CVSpilsPrecSetupFnB is identical to CVLsPrecSetupFnB, 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.

CVLsPrecSetupFnBS

Definition
```
typedef int (*CVLsPrecSetupFnBS)(realtype t, N_Vector y, N_Vector *yS,
                                 N_Vector yB, N_Vector fyB,
                                 booleantype jokB, booleantype *jcurPtrB,
                                 realtype gammaB, 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 a CVLsPrecSetupFnBS are as follows:

t	is the current value of the independent variable.

`y`	is the current value of the forward solution vector.
`yS`	is a pointer to an array containing the forward sensitivity vectors.
`yB`	is the current value of the backward dependent variable vector.
`fyB`	is the current value of the backward right-hand side function f_B.
`jokB`	is an input flag indicating whether Jacobian-related data needs to be recomputed (`jokB`=`SUNFALSE`) or information saved from a previous invokation can be safely used (`jokB`=`SUNTRUE`).
`jcurPtr`	is an output flag which must be set to `SUNTRUE` if Jacobian-relatd data was recomputed or `SUNFALSE` otherwise.
`gammaB`	is the scalar appearing in the matrix $M_B = I - \gamma_B J_B$.
`user_dataB`	is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

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 `CVSpilsPrecSetupFnBS` is identical to `CVLsPrecSetupFnBS`, 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 CVODES preconditioner modules for the backward problem

As on the forward integration phase, the efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. Both preconditioner modules provided with SUNDIALS, the serial banded preconditioner CVBANDPRE and the parallel band-block-diagonal preconditioner module CVBBDPRE, provide interface functions through which they can be used on the backward integration phase.

6.4.1 Using the banded preconditioner CVBANDPRE

The adjoint module in CVODES offers an interface to the banded preconditioner module CVBANDPRE described in section §4.8.1. This preconditioner, usable only in a serial setting, provides a band matrix preconditioner based on difference quotients of the backward problem right-hand side function `fB`. It generates a banded approximation to the Jacobian with m_{lB} sub-diagonals and m_{uB} super-diagonals to be used with one of the Krylov linear solvers.

In order to use the CVBANDPRE module in the solution of the backward problem, the user need not define any additional functions. Instead, *after* an iterative SUNLINSOL object has been attached to CVODES via a call to `CVodeSetLinearSolverB`, the following call to the CVBANDPRE module initialization function must be made.

`CVBandPrecInitB`

Call `flag = CVBandPrecInitB(cvode_mem, which, nB, muB, mlB);`

Description The function `CVBandPrecInitB` initializes and allocates memory for the CVBANDPRE preconditioner for the backward problem. It creates, allocates, and stores (internally in the CVODES solver block) a pointer to the newly created CVBANDPRE memory block.

Arguments

`cvode_mem`	(`void *`) pointer to the CVODES memory block.
`which`	(`int`) the identifier of the backward problem.
`nB`	(`sunindextype`) backward problem dimension.

`muB` (`sunindextype`) upper half-bandwidth of the backward problem Jacobian approximation.

`mlB` (`sunindextype`) lower half-bandwidth of the backward problem Jacobian approximation.

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

`CVLS_SUCCESS`	The call to `CVodeBandPrecInitB` was successful.
`CVLS_MEM_FAIL`	A memory allocation request has failed.
`CVLS_MEM_NULL`	The `cvode_mem` argument was `NULL`.
`CVLS_LMEM_NULL`	No linear solver has been attached.
`CVLS_ILL_INPUT`	An invalid parameter has been passed.

F2003 Name `FCVBandPrecInitB`

For more details on CVBANDPRE see §4.8.1.

6.4.2 Using the band-block-diagonal preconditioner CVBBDPRE

The adjoint module in CVODES offers an interface to the band-block-diagonal preconditioner module CVBBDPRE described in section §4.8.2. 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 CVBBDPRE module in the solution of the backward problem, the user must define one or two additional functions, described at the end of this section.

6.4.2.1 Initialization of CVBBDPRE

The CVBBDPRE module is initialized by calling the following function, *after* an iterative SUNLINSOL object has been attached to CVODES via a call to `CVodeSetLinearSolverB`.

`CVBBDPrecInitB`

Call
```
flag = CVBBDPrecInitB(cvode_mem, which, NlocalB, mudqB, mldqB,
                      mukeepB, mlkeepB, dqrelyB, glocB, gcommB);
```

Description The function `CVBBDPrecInitB` initializes and allocates memory for the CVBBDPRE preconditioner for the backward problem. It creates, allocates, and stores (internally in the CVODES solver block) a pointer to the newly created CVBBDPRE memory block.

Arguments

`cvode_mem` (`void *`) pointer to the CVODES 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`$= 0.0$.

`glocB` (`CVBBDLocalFnB`) the function which computes the function $g_B(t, y, y_B)$ approximating the right-hand side of the backward problem.

gcommB (CVBBDCommFnB) the optional function which performs all interprocess communication required for the computation of g_B.

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

CVLS_SUCCESS	The call to CVodeBBDPrecInitB was successful.
CVLS_MEM_FAIL	A memory allocation request has failed.
CVLS_MEM_NULL	The cvode_mem argument was NULL.
CVLS_LMEM_NULL	No linear solver has been attached.
CVLS_ILL_INPUT	An invalid parameter has been passed.

F2003 Name FCVBBDPrecInitB

To reinitialize the CVBBDPRE preconditioner module for the backward problem, possibly with changes in mudqB, mldqB, or dqrelyB, call the following function:

CVBBDPrecReInitB

Call `flag = CVBBDPrecReInitB(cvode_mem, which, mudqB, mldqB, dqrelyB);`

Description The function CVBBDPrecReInitB reinitializes the CVBBDPRE preconditioner for the backward problem.

Arguments

cvode_mem	(void *) pointer to the CVODES memory block returned by CVodeCreate.
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:

CVLS_SUCCESS	The call to CVodeBBDPrecReInitB was successful.
CVLS_MEM_FAIL	A memory allocation request has failed.
CVLS_MEM_NULL	The cvode_mem argument was NULL.
CVLS_PMEM_NULL	The CVodeBBDPrecInitB has not been previously called.
CVLS_LMEM_NULL	No linear solver has been attached.
CVLS_ILL_INPUT	An invalid parameter has been passed.

F2003 Name FCVBBDPrecReInitB

For more details on CVBBDPRE see §4.8.2.

6.4.2.2 User-supplied functions for CVBBDPRE

To use the CVBBDPRE module, the user must supply one or two functions which the module calls to construct the preconditioner: a required function glocB (of type CVBBDLocalFnB) which approximates the right-hand side of the backward problem and which is computed locally, and an optional function gcommB (of type CVBBDCommFnB) which performs all interprocess communication necessary to evaluate this approximate right-hand side (see §4.8.2). The prototypes for these two functions are described below.

CVBBDLocalFnB

Definition
```
typedef int (*CVBBDLocalFnB)(sunindextype NlocalB, realtype t, N_Vector y,
                             N_Vector yB, N_Vector gB, void *user_dataB);
```

Purpose This glocB function loads the vector gB, an approximation to the right-hand side f_B of the backward problem, as a function of t, y, and yB.

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.
- `yB` is the current value of the backward dependent variable vector.
- `gB` is the output vector, $g_B(t, y, y_B)$.
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

Return value An `CVBBDLocalFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_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 `CVBBDLocalFnB`, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the preconditioner setup function which will halt the integration (`CVodeB` returns `CV_LSETUP_FAIL`).

`CVBBDCommFnB`

Definition
```
typedef int (*CVBBDCommFnB)(sunindextype NlocalB, realtype t, N_Vector y,
                            N_Vector yB, void *user_dataB);
```

Purpose This `gcommB` function must perform all interprocess communications necessary for the execution of the `glocB` function above, using the input vectors `y` and `yB`.

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.
- `yB` is the current value of the backward dependent variable vector.
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

Return value An `CVBBDCommFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_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 right-hand side of the backward problem with the same `t`, `y`, and `yB`, arguments. If there is no additional communication needed, then pass `gcommB = NULL` to `CVBBDPrecInitB`.

Chapter 7

Using CVODES for Fortran Applications

A Fortran 2003 module (`fcvodes_mod`) is provided to support the use of CVODES, in a mixed Fortran/C setting. While CVODES 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 CVODES Fortran 2003 Interface Module

The `fcvodes_mod` Fortran module defines interfaces to most CVODES 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 CVODES function `CVodeCreate` is interfaced as `FCVodeCreate`. Thus, the steps to use CVODES 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 CVODES interface module can be accessed by the `use` statement, i.e. `use fcvodes_mod`, and linking to the library `libsundials_fcvodes_mod.`*lib* in addition to `libsundials_cvodes.`*lib*.

The Fortran 2003 interface modules were generated with SWIG Fortran, a fork of SWIG [36]. 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 8, 9, 10, and 11 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.

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.

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)

7.1.3.1 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 8.1.5.

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.

`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

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.

8.1 The NVECTOR API

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

8.1.1 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 8.1.

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`. This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, the sparse linear solvers (serial and threaded), and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS.

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

Return value `realtype*`

F2003 Name `FN_VGetArrayPointer`

`N_VSetArrayPointer`

Call `N_VSetArrayPointer(vdata, v);`

Description Overwrites the pointer to the data in an `N_Vector` with a given `realtype*`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype`. This routine is only used in the interfaces to the dense (serial) linear solver, hence need not exist in a user-supplied NVECTOR module for a parallel environment.

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

Return value None

F2003 Name `FN_VSetArrayPointer`

`N_VGetCommunicator`

Call `N_VGetCommunicator(v);`

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

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

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

F2003 Name `FN_VGetCommunicator`

`N_VGetLength`

Call `N_VGetLength(v);`

Description Returns the global length (number of 'active' entries) in the NVECTOR `v`. This value should be cumulative across all processes if the vector is used in a parallel environment. If `v` contains additional storage, e.g., for parallel communication, those entries should not be included.

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

Return value `sunindextype`

F2003 Name `FN_VGetLength`

`N_VLinearSum`

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

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

Arguments `a` (`realtype`) constant that scales `x`

`x` (`N_Vector`) a NVECTOR object

`b` (`realtype`) constant that scales `y`

`y` (`N_Vector`) a NVECTOR object

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

Return value None

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`: $y_i = |x_i|$, $i = 0, \ldots, n-1$.

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

Return value None

F2003 Name `FN_VAbs`

`N_VInv`

Call `N_VInv(x, z);`

Description Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$. This routine may not check for division by 0. It should be called only with an `x` which is guaranteed to have all nonzero components.

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

Return value None

F2003 Name `FN_VInv`

`N_VAddConst`

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

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

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

Return value None

F2003 Name `FN_VAddConst`

`N_VDotProd`

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

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

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

Return value `realtype`

F2003 Name `FN_VDotProd`

`N_VMaxNorm`

Call `m = N_VMaxNorm(x);`

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

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

Return value `realtype`

F2003 Name `FN_VMaxNorm`

`N_VWrmsNorm`

Call `m = N_VWrmsNorm(x, w)`

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

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

Return value `realtype`

F2003 Name `FN_VWrmsNorm`

`N_VWrmsNormMask`

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

Description Returns the weighted root mean square norm of the `N_Vector x` with `realtype` weight vector `w` built using only the elements of `x` corresponding to positive elements of the `N_Vector id`: $m = \sqrt{\left(\sum_{i=0}^{n-1}(x_i w_i H(id_i))^2\right)/n}$, where $H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$

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

Return value `realtype`

F2003 Name `FN_VWrmsNormMask`

`N_VMin`

Call `m = N_VMin(x);`

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

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

Return value `realtype`

F2003 Name `FN_VMin`

`N_VWL2Norm`

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

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

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

Return value `realtype`

F2003 Name `FN_VWL2Norm`

`N_VL1Norm`

Call `m = N_VL1Norm(x);`

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

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

Return value `realtype`

F2003 Name `FN_VL1Norm`

N_VCompare

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

Description Compares the components of the `N_Vector x` to the `realtype` scalar `c` and returns an `N_Vector z` such that: $z_i = 1.0$ if $|x_i| \geq c$ and $z_i = 0.0$ otherwise.

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

Return value None

F2003 Name `FN_VCompare`

N_VInvTest

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

Description Sets the components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`, with prior testing for zero values: $z_i = 1.0/x_i$, $i = 0, \ldots, n-1$.

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

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

F2003 Name `FN_VInvTest`

N_VConstrMask

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

Description Performs the following constraint tests: $x_i > 0$ if $c_i = 2$, $x_i \geq 0$ if $c_i = 1$, $x_i \leq 0$ if $c_i = -1$, $x_i < 0$ if $c_i = -2$. There is no constraint on x_i if $c_i = 0$. This routine returns a boolean assigned to `SUNFALSE` if any element failed the constraint test and assigned to `SUNTRUE` if all passed. It also sets a mask vector `m`, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.

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

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

F2003 Name `FN_VConstrMask`

N_VMinQuotient

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

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

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

Return value `realtype`

F2003 Name `FN_VMinQuotient`

8.1.2 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)
```

8.1.3 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:

$$z_{j,i} = a x_{j,i} + b y_{j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$

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:

$$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, n_v - 1,$$

where c is an array of n_s scalars, 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.

8.1.4 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 8.14). If a particular NVECTOR implementation defines a local reduction operation as `NULL`, the NVECTOR_MPIMANYVECTOR module will automatically call standard vector reduction operations as necessary to complete the desired operation. All SUNDIALS-provided NVECTOR implementations include these local reduction operations, which may be used as templates for user-defined NVECTOR implementations.

`N_VDotProdLocal`

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

Description This routine computes the MPI task-local portion of the ordinary dot product of `x` and `y`:

$$d = \sum_{i=0}^{n_{local}-1} x_i y_i,$$

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

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

Return value `realtype`

F2003 Name `FN_VDotProdLocal`

`N_VMaxNormLocal`

Call `m = N_VMaxNormLocal(x);`

Description This routine computes the MPI task-local portion of the maximum norm of the `N_Vector` `x`:

$$m = \max_{0 \le i < n_{local}} |x_i|,$$

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

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

Return value `realtype`

F2003 Name `FN_VMaxNormLocal`

`N_VMinLocal`

Call `m = N_VMinLocal(x);`

Description This routine computes the smallest element of the MPI task-local portion of the `N_Vector x`:

$$m = \min_{0 \le i < n_{local}} x_i,$$

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

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

Return value `realtype`

F2003 Name `FN_VMinLocal`

`N_VL1NormLocal`

Call `n = N_VL1NormLocal(x);`

Description This routine computes the MPI task-local portion of the ℓ_1 norm of the `N_Vector x`:

$$n = \sum_{i=0}^{n_{local}-1} |x_i|,$$

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

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

Return value `realtype`

F2003 Name `FN_VL1NormLocal`

`N_VWSqrSumLocal`

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

Description This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector x` with weight vector `w`:

$$s = \sum_{i=0}^{n_{local}-1} (x_i w_i)^2,$$

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

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

Return value `realtype`

F2003 Name `FN_VWSqrSumLocal`

`N_VWSqrSumMaskLocal`

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

Description This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector x` with weight vector `w` built using only the elements of `x` corresponding to positive elements of the `N_Vector id`:

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

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

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

Return value `realtype`

F2003 Name `FN_VWSqrSumMaskLocal`

`N_VInvTestLocal`

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

Description Sets the MPI task-local components of the `N_Vector z` to be the inverses of the components of the `N_Vector x`, with prior testing for zero values:

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

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

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

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

F2003 Name `FN_VInvTestLocal`

`N_VConstrMaskLocal`

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

Description Performs the following constraint tests:

$$\begin{aligned} x_i > 0 \quad &\text{if} \quad c_i = 2, \\ x_i \geq 0 \quad &\text{if} \quad c_i = 1, \\ x_i \leq 0 \quad &\text{if} \quad c_i = -1, \\ x_i < 0 \quad &\text{if} \quad c_i = -2, \text{and} \\ \text{no test} \quad &\text{if} \quad c_i = 0, \end{aligned}$$

for all MPI task-local components of the vectors. It sets a mask vector `m`, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.

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

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

F2003 Name `FN_VConstrMaskLocal`

`N_VMinQuotientLocal`

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

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

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

Return value `realtype`

F2003 Name `FN_VMinQuotientLocal`

8.1.5 NVECTOR utility functions

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

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

`N_VNewEmpty`

Call `v = N_VNewEmpty();`

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

Arguments None

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

F2003 Name `FN_VNewEmpty`

`N_VCopyOps`

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

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

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

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

F2003 Name `FN_VCopyOps`

`N_VFreeEmpty`

Call `N_VFreeEmpty(v);`

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

Arguments `v` (`N_Vector`)

Return value None

F2003 Name `FN_VFreeEmpty`

`N_VCloneEmptyVectorArray`

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

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

Arguments `count` (`int`) the size of the vector array
`w` (`N_Vector`) the vector to clone

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

`N_VCloneVectorArray`

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

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

Arguments `count` (`int`) the size of the vector array
`w` (`N_Vector`) the vector to clone

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

`N_VDestroyVectorArray`

Call `N_VDestroyVectorArray(count, w);`

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

Arguments `vs` (`N_Vector*`) the array of vectors to destroy
`count` (`int`) the size of the vector array

Return value None

`N_VNewVectorArray`

Call `vecarray = N_VNewVectorArray(count);`

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

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

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

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

F2003 Name `FN_VNewVectorArray`

Table 8.1: Vector Identifications associated with vector kernels supplied with SUNDIALS.

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

`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`

8.1.6 NVECTOR identifiers

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 8.1.

8.1.7 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);
  void         (*nvsetarraypointer)(realtype *, N_Vector);
  void*        (*nvgetcommunicator)(N_Vector);
  sunindextype (*nvgetlength)(N_Vector);
  void         (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
  void         (*nvconst)(realtype, N_Vector);
  void         (*nvprod)(N_Vector, N_Vector, N_Vector);
  void         (*nvdiv)(N_Vector, N_Vector, N_Vector);
  void         (*nvscale)(realtype, N_Vector, N_Vector);
  void         (*nvabs)(N_Vector, N_Vector);
  void         (*nvinv)(N_Vector, N_Vector);
  void         (*nvaddconst)(N_Vector, realtype, N_Vector);
  realtype     (*nvdotprod)(N_Vector, N_Vector);
  realtype     (*nvmaxnorm)(N_Vector);
  realtype     (*nvwrmsnorm)(N_Vector, N_Vector);
  realtype     (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
  realtype     (*nvmin)(N_Vector);
  realtype     (*nvwl2norm)(N_Vector, N_Vector);
  realtype     (*nvl1norm)(N_Vector);
  void         (*nvcompare)(realtype, N_Vector, N_Vector);
  booleantype  (*nvinvtest)(N_Vector, N_Vector);
  booleantype  (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
  realtype     (*nvminquotient)(N_Vector, N_Vector);
  int          (*nvlinearcombination)(int, realtype*, N_Vector*, N_Vector);
  int          (*nvscaleaddmulti)(int, realtype*, N_Vector, N_Vector*, N_Vector*);
  int          (*nvdotprodmulti)(int, N_Vector, N_Vector*, realtype*);
  int          (*nvlinearsumvectorarray)(int, realtype, N_Vector*, realtype,
                                         N_Vector*, N_Vector*);
  int          (*nvscalevectorarray)(int, realtype*, N_Vector*, N_Vector*);
  int          (*nvconstvectorarray)(int, realtype, N_Vector*);
  int          (*nvwrmsnomrvectorarray)(int, N_Vector*, N_Vector*, realtype*);
  int          (*nvwrmsnomrmaskvectorarray)(int, N_Vector*, N_Vector*, N_Vector,
                                            realtype*);
  int          (*nvscaleaddmultivectorarray)(int, int, realtype*, N_Vector*,
                                             N_Vector**, N_Vector**);
  int          (*nvlinearcombinationvectorarray)(int, int, realtype*, N_Vector**,
                                                 N_Vector*);
  realtype     (*nvdotprodlocal)(N_Vector, N_Vector);
  realtype     (*nvmaxnormlocal)(N_Vector);
```

```
  realtype     (*nvminlocal)(N_Vector);
  realtype     (*nvl1normlocal)(N_Vector);
  booleantype  (*nvinvtestlocal)(N_Vector, N_Vector);
  booleantype  (*nvconstrmasklocal)(N_Vector, N_Vector, N_Vector);
  realtype     (*nvminquotientlocal)(N_Vector, N_Vector);
  realtype     (*nvwsqrsumlocal)(N_Vector, N_Vector);
  realtype     (*nvwsqrsummasklocal(N_Vector, N_Vector, N_Vector);

};
```

The generic NVECTOR module defines and implements the vector operations acting on an `N_Vector`. These routines are nothing but wrappers for the vector operations defined by a particular NVECTOR implementation, which are accessed through the *ops* field of the `N_Vector` structure. To illustrate this point we show below the implementation of a typical vector operation from the generic NVECTOR module, namely `N_VScale`, which performs the scaling of a vector `x` by a scalar `c`:

```
void N_VScale(realtype c, N_Vector x, N_Vector z)
{
   z->ops->nvscale(c, x, z);
}
```

Section 8.1.1 defines a complete list of all standard vector operations defined by the generic NVECTOR module. Sections 8.1.2, 8.1.3 and 8.1.4 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
 end type N_Vector_Ops
```

8.1.8 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.

8.1.8.1 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 8.1.1-8.1.4 above naturally extend to complex-valued vectors; however, some do not. To this end, we provide the following guidance:

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

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

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

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

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

8.2 NVECTOR functions used by CVODES

In Table 8.2 below, we list the vector functions in the NVECTOR module used within the CVODES package. The table also shows, for each function, which of the code modules uses the function. The CVODES column shows function usage within the main integrator module, while the remaining columns show function usage within each of the CVODES linear solver interfaces, the CVBANDPRE and CVBBDPRE preconditioner modules, and the CVODES adjoint sensitivity module (denoted here by CVODEA). Here CVLS stands for the generic linear solver interface in CVODES, and CVDIAG stands for the diagonal linear solver interface in CVODES.

At this point, we should emphasize that the CVODES user does not need to know anything about the usage of vector functions by the CVODES code modules in order to use CVODES. 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 CVODES modules for user feedback.
3. The optional function `N_VDotProdMulti` is only used in the SUNNONLINSOL_FIXEDPOINT module, or when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR.
4. This routine is only used when an iterative or matrix iterative SUNLINSOL module is supplied to CVODES.

Each SUNLINSOL object may require additional NVECTOR routines not listed in the table above. Please see the the relevant descriptions of these modules in Sections 10.5-10.17 for additional detail on their NVECTOR requirements.

The remaining operations from Tables 8.1.1, 8.1.2, and 8.1.3 not listed above are unused and a user-supplied NVECTOR module for CVODES could omit these operations (although some may be needed by SUNNONLINSOL or SUNLINSOL modules). The functions `N_MinQuotient`, `N_VConstrMask`, and `N_VCompare` are only used when constraint checking is enabled and may be omitted if this feature is not used.

8.3 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.

8.3.1 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] )
  ```

8.3.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3 and 8.1.4. 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 8.1.1 with the suffix `_Serial` appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. `FN_VDestroy_Serial`).

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

`N_VNew_Serial`

Prototype `N_Vector N_VNew_Serial(sunindextype vec_length);`

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

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

`N_VNewEmpty_Serial`

Prototype `N_Vector N_VNewEmpty_Serial(sunindextype vec_length);`

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

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

`N_VMake_Serial`

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

Description This function creates and allocates memory for a serial vector with user-provided data array.

(This function does *not* allocate memory for `v_data` itself.)

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

`N_VCloneVectorArray_Serial`

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

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

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

`N_VCloneVectorArrayEmpty_Serial`

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

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

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

`N_VDestroyVectorArray_Serial`

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

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

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

`N_VPrint_Serial`

Prototype `void N_VPrint_Serial(N_Vector v);`

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

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

`N_VPrintFile_Serial`

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

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

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

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

`N_VEnableFusedOps_Serial`

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

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

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

`N_VEnableLinearCombination_Serial`

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

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

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

`N_VEnableScaleAddMulti_Serial`

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

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

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

`N_VEnableDotProdMulti_Serial`

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

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

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

`N_VEnableLinearSumVectorArray_Serial`

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

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

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

`N_VEnableScaleVectorArray_Serial`

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

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

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

`N_VEnableConstVectorArray_Serial`

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

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

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

`N_VEnableWrmsNormVectorArray_Serial`

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

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

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

`N_VEnableWrmsNormMaskVectorArray_Serial`

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

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

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

`N_VEnableScaleAddMultiVectorArray_Serial`

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

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

`N_VEnableLinearCombinationVectorArray_Serial`

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

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

Notes

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

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

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

8.3.3 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.

8.4 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.

8.4.1 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] )
  ```

8.4.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4. Their names are obtained from those in these tables by appending the suffix _Parallel (e.g. N_VDestroy_Parallel). The module NVECTOR_PARALLEL provides the following additional user-callable routines:

N_VNew_Parallel

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

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

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

`N_VNewEmpty_Parallel`

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

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

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

`N_VMake_Parallel`

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

Description This function creates and allocates memory for a parallel vector with user-provided data array. This function does *not* allocate memory for `v_data` itself.

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

`N_VCloneVectorArray_Parallel`

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

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

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

`N_VCloneVectorArrayEmpty_Parallel`

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

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

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

`N_VDestroyVectorArray_Parallel`

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

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

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

`N_VGetLocalLength_Parallel`

Prototype `sunindextype N_VGetLocalLength_Parallel(N_Vector v);`

Description This function returns the local vector length.

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

`N_VPrint_Parallel`

Prototype `void N_VPrint_Parallel(N_Vector v);`

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

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

`N_VPrintFile_Parallel`

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

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

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

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

`N_VEnableFusedOps_Parallel`

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

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

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

`N_VEnableLinearCombination_Parallel`

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

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

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

`N_VEnableScaleAddMulti_Parallel`

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

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

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

`N_VEnableDotProdMulti_Parallel`

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

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

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

`N_VEnableLinearSumVectorArray_Parallel`

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

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

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

`N_VEnableScaleVectorArray_Parallel`

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

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

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

`N_VEnableConstVectorArray_Parallel`

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

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

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

`N_VEnableWrmsNormVectorArray_Parallel`

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

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

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

`N_VEnableWrmsNormMaskVectorArray_Parallel`

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

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

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

`N_VEnableScaleAddMultiVectorArray_Parallel`

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

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

`N_VEnableLinearCombinationVectorArray_Parallel`

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

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

Notes

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

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

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

8.4.3 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.

8.5 The NVECTOR_OPENMP implementation

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

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

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

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

8.5.1 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] )
  ```

8.5.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4. 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 8.1.1 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.

8.5.3 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.

8.6 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.

8.6.1 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] )
  ```

8.6.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4. 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 8.1.1 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.

8.6.3 NVECTOR_PTHREADS Fortran interfaces

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

FORTRAN 2003 interface module

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

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

FORTRAN 77 interface functions

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

8.7 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.

8.7.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 [33] and the `ark_diurnal_kry_ph.c` example program for ARKODE [46].

The names of parhyp methods are obtained from those in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR_PARHYP provides the following additional user-callable routines:

`N_VNewEmpty_ParHyp`

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

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

`N_VMake_ParHyp`

Prototype `N_Vector N_VMake_ParHyp(HYPRE_ParVector x)`

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

`N_VGetVector_ParHyp`

Prototype `HYPRE_ParVector N_VGetVector_ParHyp(N_Vector v)`

Description This function returns the underlying *hypre* vector.

`N_VCloneVectorArray_ParHyp`

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

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

`N_VCloneVectorArrayEmpty_ParHyp`

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

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

`N_VDestroyVectorArray_ParHyp`

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

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

`N_VPrint_ParHyp`

Prototype `void N_VPrint_ParHyp(N_Vector v)`

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

`N_VPrintFile_ParHyp`

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

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

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

`N_VEnableFusedOps_ParHyp`

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

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

`N_VEnableLinearCombination_ParHyp`

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

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

`N_VEnableScaleAddMulti_ParHyp`

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

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

`N_VEnableDotProdMulti_ParHyp`

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

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

`N_VEnableLinearSumVectorArray_ParHyp`

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

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

`N_VEnableScaleVectorArray_ParHyp`

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

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

N_VEnableConstVectorArray_ParHyp

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

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

N_VEnableWrmsNormVectorArray_ParHyp

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

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

N_VEnableWrmsNormMaskVectorArray_ParHyp

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

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

N_VEnableScaleAddMultiVectorArray_ParHyp

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

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

N_VEnableLinearCombinationVectorArray_ParHyp

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

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

Notes

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

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

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

8.8 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.

8.8.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 [32].

The names of vector operations are obtained from those in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4 by appending the suffix `_Petsc` (e.g. `N_VDestroy_Petsc`). The module NVECTOR_PETSC provides the following additional user-callable routines:

`N_VNewEmpty_Petsc`

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

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

`N_VMake_Petsc`

Prototype `N_Vector N_VMake_Petsc(Vec *pvec)`

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

`N_VGetVector_Petsc`

Prototype `Vec *N_VGetVector_Petsc(N_Vector v)`

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

`N_VCloneVectorArray_Petsc`

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

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

`N_VCloneVectorArrayEmpty_Petsc`

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

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

`N_VDestroyVectorArray_Petsc`

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

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

`N_VPrint_Petsc`

Prototype `void N_VPrint_Petsc(N_Vector v)`

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

`N_VPrintFile_Petsc`

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

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

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

`N_VEnableFusedOps_Petsc`

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

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

`N_VEnableLinearCombination_Petsc`

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

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

`N_VEnableScaleAddMulti_Petsc`

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

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

`N_VEnableDotProdMulti_Petsc`

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

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

`N_VEnableLinearSumVectorArray_Petsc`

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

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

`N_VEnableScaleVectorArray_Petsc`

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

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

`N_VEnableConstVectorArray_Petsc`

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

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

`N_VEnableWrmsNormVectorArray_Petsc`

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

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

`N_VEnableWrmsNormMaskVectorArray_Petsc`

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

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

`N_VEnableScaleAddMultiVectorArray_Petsc`

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

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

`N_VEnableLinearCombinationVectorArray_Petsc`

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

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

Notes

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

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

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

8.9 The NVECTOR_CUDA implementation

The NVECTOR_CUDA module is an experimental NVECTOR implementation in the CUDA language. The module allows for SUNDIALS vector kernels to run on GPU devices. It is intended for users who are already familiar with CUDA and GPU programming. Building this vector module requires a CUDA compiler and, by extension, a C++ compiler. The class `Vector` in the namespace `suncudavec` manages the vector data layout:

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

The class members are vector size (length), size of the vector data memory block, pointers to vector data on the host and the device, pointers to `ThreadPartitioning` implementations that handle thread

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

```
struct _N_VectorContent_Cuda {};
```

to interface the C++ class with the NVECTOR C code. Due to the rapid progress of CUDA development, we expect that the `suncudavec::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `suncudavec::Vector` class without requiring changes to the user API.

When instantiated with `N_VNew_Cuda`, the class `Vector` will allocate memory on both the host and the device. Alternatively, a user can provide host and device data arrays by using the `N_VMake_Cuda` constructor. To use CUDA managed memory, the constructors `N_VNewManaged_Cuda` and `N_VMakeManaged_Cuda` are provided. Details on each of these constructors are provided below.

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.

8.9.1 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_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 8.1.1, 8.1.2, 8.1.3 and 8.1.4, except for `N_VSetArrayPointer`, and, if using unmanaged memory, `N_VGetArrayPointer`. 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 [33].

The names of vector operations are obtained from those in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4 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_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.

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

`N_VSetCudaStream_Cuda`

Prototype `void N_VSetCudaStream_Cuda(N_Vector v, cudaStream_t *stream)`

Description This function sets the CUDA stream that all vector kernels will be launched on. By default an NVECTOR_CUDA uses the default CUDA stream.

Note: All vectors used in a single instance of a SUNDIALS solver must use the same CUDA *stream, and the* CUDA *stream must be set prior to solver initialization. Additionally, if manually instantiating the stream and reduce* `ThreadPartitioning` *of a* `suncudavec::Vector`*, ensure that they use the same* CUDA *stream.*

`N_VCopyToDevice_Cuda`

Prototype `void N_VCopyToDevice_Cuda(N_Vector v)`

Description This function copies host vector data to the device.

`N_VCopyFromDevice_Cuda`

Prototype `void N_VCopyFromDevice_Cuda(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VPrint_Cuda`

Prototype `void N_VPrint_Cuda(N_Vector v)`

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

`N_VPrintFile_Cuda`

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

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

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

`N_VEnableFusedOps_Cuda`

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

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

`N_VEnableLinearCombination_Cuda`

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

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

`N_VEnableScaleAddMulti_Cuda`

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

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

`N_VEnableDotProdMulti_Cuda`

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

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

`N_VEnableLinearSumVectorArray_Cuda`

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

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

`N_VEnableScaleVectorArray_Cuda`

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

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

`N_VEnableConstVectorArray_Cuda`

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

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

`N_VEnableWrmsNormVectorArray_Cuda`

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

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

`N_VEnableWrmsNormMaskVectorArray_Cuda`

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

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

`N_VEnableScaleAddMultiVectorArray_Cuda`

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

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

`N_VEnableLinearCombinationVectorArray_Cuda`

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

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

Notes

- When there is a need to access components of an `N_Vector_Cuda`, `v`, it is recommeded to use functions `N_VGetDeviceArrayPointer_Cuda` or `N_VGetHostArrayPointer_Cuda`. However, when using managed memory, the function `N_VGetArrayPointer` may also be used.

- 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.

8.10 The NVECTOR_RAJA implementation

The NVECTOR_RAJA module is an experimental NVECTOR implementation using the RAJA hardware abstraction layer. In this implementation, RAJA allows for SUNDIALS vector kernels to run on GPU devices. The module is intended for users who are already familiar with RAJA and GPU programming. Building this vector module requires a C++11 compliant compiler and a CUDA software development toolkit. Besides the CUDA backend, RAJA has other backends such as serial, OpenMP, and OpenACC. These backends are not used in this SUNDIALS release. Class `Vector` in namespace `sunrajavec` manages the vector data layout:

```
template <class T, class I>
class Vector {
   I size_;
   I mem_size_;
   T* h_vec_;
   T* d_vec_;
  ...
};
```

The class members are: vector size (length), size of the vector data memory block, the global vector size (length), a pointer to the vector data on the host, and a pointer to the vector data on the device. The class `Vector` inherits from an empty structure

```
struct _N_VectorContent_Raja { };
```

to interface the C++ class with the NVECTOR C code. When instantiated, the class `Vector` will allocate memory on both the host and the device. Due to the rapid progress of RAJA development, we expect that the `sunrajavec::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `sunrajavec::Vector` class without requiring changes to the user API.

The header file to include when using this module is `nvector_raja.h`. The installed module library to link to are `libsundials_nveccudaraja.`*`lib`*. The extension *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

8.10.1 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.

The NVECTOR_RAJA module defines the implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 implemented by the RAJA vector. As such, this vector cannot be used with the SUNDIALS Fortran interfaces, nor with the SUNDIALS direct solvers and preconditioners. The NVECTOR_RAJA module provides separate functions to access data on the host and on the device. It also provides methods for copying data from the host to the device and vice versa. Usage examples of NVECTOR_RAJA are provided in some example programs for CVODE [33].

The names of vector operations are obtained from those in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4 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 CUDA `N_Vector`. The vector data array is allocated on both the host and device.

`N_VNewEmpty_Raja`

Prototype `N_Vector N_VNewEmpty_Raja()`

Description This function creates a new NVECTOR wrapper with the pointer to the wrapped RAJA vector set to `NULL`. It is used by the `N_VNew_Raja`, `N_VMake_Raja`, and `N_VClone_Raja` implementations.

`N_VMake_Raja`

Prototype `N_Vector N_VMake_Raja(N_VectorContent_Raja c)`

Description This function creates and allocates memory for an NVECTOR_RAJA wrapper around a user-provided `sunrajavec::Vector` class. Its only argument is of type `N_VectorContent_Raja`, which is the pointer to the class.

`N_VCopyToDevice_Raja`

Prototype `realtype *N_VCopyToDevice_Raja(N_Vector v)`

Description This function copies host vector data to the device.

`N_VCopyFromDevice_Raja`

Prototype `realtype *N_VCopyFromDevice_Raja(N_Vector v)`

Description This function copies vector data from the device to the host.

`N_VPrint_Raja`

Prototype `void N_VPrint_Raja(N_Vector v)`

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

`N_VPrintFile_Raja`

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

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

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

`N_VEnableFusedOps_Raja`

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

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

`N_VEnableLinearCombination_Raja`

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

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

`N_VEnableScaleAddMulti_Raja`

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

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

`N_VEnableLinearSumVectorArray_Raja`

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

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

`N_VEnableScaleVectorArray_Raja`

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

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

`N_VEnableConstVectorArray_Raja`

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

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

N_VEnableScaleAddMultiVectorArray_Raja

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

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

N_VEnableLinearCombinationVectorArray_Raja

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

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

Notes

- When there is a need to access components of an N_Vector_Raja, v, it is recommeded to use functions N_VGetDeviceArrayPointer_Raja or N_VGetHostArrayPointer_Raja.

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

8.11 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.

8.11.1 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 )
  ```

8.11.2 NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 8.1.1, 8.1.2, 8.1.3, and 8.1.4 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.

8.12 The NVECTOR_TRILINOS implementation

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

```
struct _N_VectorContent_Trilinos {};
```

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

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

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

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

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

8.12.1 NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in Tables 8.1.1, 8.1.4, and 8.1.4, 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 [32].

The names of vector operations are obtained from those in Tables 8.1.1, 8.1.4, and 8.1.4 by appending the suffix _Trilinos (e.g. N_VDestroy_Trilinos). Vector operations call existing Tpetra::Vector methods when available. Vector operations specific to SUNDIALS are implemented as standalone functions in the namespace Sundials::TpetraVector, located in the file SundialsTpetraVectorKernels.hpp. The module NVECTOR_TRILINOS provides the following additional user-callable functions:

- N_VGetVector_Trilinos

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

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

- `N_VMake_Trilinos`

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

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

Notes

- The template parameter `vector_type` should be set as:
  `typedef Sundials::TpetraVectorInterface::vector_type vector_type`
  This will ensure that data types used in Tpetra vector match those in SUNDIALS.
- When there is a need to access components of an `N_Vector_Trilinos`, `v`, it is recommeded to extract the Trilinos vector object via `x_vec = N_VGetVector_Trilinos(v)` and then access components using the appropriate Trilinos functions.
- The functions `N_VDestroy_Trilinos` and `N_VDestroyVectorArray_Trilinos` only delete the `N_Vector` wrapper. The underlying Tpetra vector object will exist for as long as there is at least one reference to it.

8.13 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.

8.13.1 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.

8.13.2 NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 8.1.1, 8.1.2, 8.1.3, and 8.1.4 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 8.1.5.

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

`N_VGetSubvector_ManyVector`

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

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

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

`N_VGetSubvectorArrayPointer_ManyVector`

Prototype `realtype *N_VGetSubvectorArrayPointer_ManyVector(N_Vector v, sunindextype vec_num);`

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

If the input `vec_num` is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then `NULL` is returned.

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

`N_VSetSubvectorArrayPointer_ManyVector`

Prototype `int N_VSetSubvectorArrayPointer_ManyVector(realtype *v_data, N_Vector v, sunindextype vec_num);`

Description This function sets the data array pointer for the `vec_num` subvector from the NVECTOR array.

If the input `vec_num` is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then this routine returns `-1`; otherwise it returns `0`.

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

`N_VGetNumSubvectors_ManyVector`

Prototype `sunindextype N_VGetNumSubvectors_ManyVector(N_Vector v);`

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

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

By default all fused and vector array operations are disabled in the NVECTOR_MANYVECTOR module, except for `N_VWrmsNormVectorArray` and `N_VWrmsNormMaskVectorArray`, that are enabled by default. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_ManyVector`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees that the new vectors will have the same operations enabled/disabled, since cloned vectors inherit those configuration options from the vector they are cloned from, while vectors created with `N_VNew_ManyVector` will have the default settings for the NVECTOR_MANYVECTOR module. We note that these routines *do not* call the corresponding routines on subvectors, so those should be set up as desired *before* attaching them to the ManyVector in `N_VNew_ManyVector`.

`N_VEnableFusedOps_ManyVector`

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

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

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

`N_VEnableLinearCombination_ManyVector`

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

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

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

`N_VEnableScaleAddMulti_ManyVector`

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

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

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

`N_VEnableDotProdMulti_ManyVector`

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

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

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

`N_VEnableLinearSumVectorArray_ManyVector`

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

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

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

`N_VEnableScaleVectorArray_ManyVector`

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

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

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

`N_VEnableConstVectorArray_ManyVector`

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

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

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

`N_VEnableWrmsNormVectorArray_ManyVector`

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

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

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

`N_VEnableWrmsNormMaskVectorArray_ManyVector`

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

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

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

Notes

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

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

8.14 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 8.1.4.

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.

8.14.1 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.

8.14.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, 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 8.1.1, 8.1.2, 8.1.3, and 8.1.4 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 8.1.5.

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

N_VMake_MPIManyVector

Prototype
```
N_Vector N_VMake_MPIManyVector(MPI_Comm comm, sunindextype num_subvectors,
                               N_Vector *vec_array);
```

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

The input comm should be this user-created MPI communicator. This routine will internally call MPI_Comm_dup to create a copy of the input comm, so the user-supplied comm argument need not be retained after the call to N_VMake_MPIManyVector.

If all subvectors are MPI-unaware, then the input comm argument should be MPI_COMM_NULL, although in this case, it would be simpler to call N_VNew_MPIManyVector instead, or to just use the NVECTOR_MANYVECTOR module.

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

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

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

`N_VGetSubvector_MPIManyVector`

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

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

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

`N_VGetSubvectorArrayPointer_MPIManyVector`

Prototype `realtype *N_VGetSubvectorArrayPointer_MPIManyVector(N_Vector v, sunindextype vec_num);`

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

If the input `vec_num` is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then `NULL` is returned.

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

`N_VSetSubvectorArrayPointer_MPIManyVector`

Prototype `int N_VSetSubvectorArrayPointer_MPIManyVector(realtype *v_data, N_Vector v, sunindextype vec_num);`

Description This function sets the data array pointer for the `vec_num` subvector from the NVECTOR array.

If the input `vec_num` is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then this routine returns `-1`; otherwise it returns `0`.

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

`N_VGetNumSubvectors_MPIManyVector`

Prototype `sunindextype N_VGetNumSubvectors_MPIManyVector(N_Vector v);`

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

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

By default all fused and vector array operations are disabled in the NVECTOR_MPIMANYVECTOR module, except for `N_VWrmsNormVectorArray` and `N_VWrmsNormMaskVectorArray`, that are enabled by default. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_MPIManyVector` or `N_VMake_MPIManyVector`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone`. This guarantees that the new vectors will have the same operations enabled/disabled, since cloned vectors inherit those configuration options from the vector they are cloned from, while vectors created with `N_VNew_MPIManyVector` and `N_VMake_MPIManyVector` will have the default settings for the NVECTOR_MPIMANYVECTOR module. We note that these routines *do not* call the corresponding routines on subvectors, so those should be set up as desired *before* attaching them to the MPIManyVector in `N_VNew_MPIManyVector` or `N_VMake_MPIManyVector`.

`N_VEnableFusedOps_MPIManyVector`

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

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

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

`N_VEnableLinearCombination_MPIManyVector`

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

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

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

`N_VEnableScaleAddMulti_MPIManyVector`

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

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

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

`N_VEnableDotProdMulti_MPIManyVector`

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

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

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

`N_VEnableLinearSumVectorArray_MPIManyVector`

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

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

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

`N_VEnableScaleVectorArray_MPIManyVector`

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

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

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

`N_VEnableConstVectorArray_MPIManyVector`

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

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

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

`N_VEnableWrmsNormVectorArray_MPIManyVector`

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

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

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

`N_VEnableWrmsNormMaskVectorArray_MPIManyVector`

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

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

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

Notes

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

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

8.15 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.

8.15.1 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 8.14.1.

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.

8.15.2 NVECTOR_MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in Tables 8.1.1, 8.1.2, 8.1.3, and 8.1.4, from the NVECTOR_MPIMANYVECTOR (see section 8.14.2) except for `N_VGetArrayPointer` and `N_VSetArrayPointer`; the module provides its own implementation of these functions that call the local vector implementations. Therefore, the NVECTOR_MPIPLUSX module implements all of the operations listed in the referenced sections except for `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray` Accordingly, it's compatibility with the SUNDIALS Fortran-77 interface, and with the SUNDIALS direct solvers and preconditioners depends on the local vector implementation.

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

`N_VMake_MPIPlusX`

Prototype
```
N_Vector N_VMake_MPIPlusX(MPI_Comm comm,
                          N_Vector *local_vector);
```

Description This function creates an MPIPlusX vector from an existing local (i.e. on-node) NVECTOR object, and a user-created MPI communicator.

The input `comm` should be this user-created MPI communicator. This routine will internally call `MPI_Comm_dup` to create a copy of the input `comm`, so the user-supplied `comm` argument need not be retained after the call to `N_VMake_MPIPlusX`.

This routine will copy the `N_Vector` pointer to the input `local_vector`, so the underlying local NVECTOR object should not be destroyed before the mpiplusx that contains it.

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

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

`N_VGetLocalVector_MPIPlusX`

Prototype
```
N_Vector N_VGetLocalVector_MPIPlusX(N_Vector v);
```

Description This function returns the local vector underneath the the MPIPlusX NVECTOR.

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

`N_VGetArrayPointer_MPIPlusX`

Prototype
```
realtype* N_VGetLocalVector_MPIPlusX(N_Vector v);
```

Description This function returns the data array pointer for the local vector if the local vector implements the `N_VGetArrayPointer` operation; otherwise it returns `NULL`.

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

`N_VSetArrayPointer_MPIPlusX`

Prototype `void N_VSetArrayPointer_MPIPlusX(realtype *data, N_Vector v);`

Description This function sets the data array pointer for the local vector if the local vector implements the `N_VSetArrayPointer` operation.

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

The NVECTOR_MPIPLUSX module does not implement any fused or vector array operations. Instead users should enable/disable fused operations on the local vector.

Notes

- `N_VMake_MPIPlusX` sets the field *own_data* = `SUNFALSE`.
  and `N_VDestroy_MPIPlusX` will not call `N_VDestroy` on the local vector. In this case, it is the user's responsibility to deallocate the local vector.

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

8.16 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 8.2: List of vector functions usage by CVODES code modules

	CVODES	CVLS	CVDIAG	CVBANDPRE	CVBBDPRE	CVODEA
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_MinQuotient	✓					
N_VConstrMask	✓					
N_VCompare	✓		✓			
N_VInvTest			✓			
N_VLinearCombination	✓					
N_VScaleAddMulti	✓					
N_VDotProdMulti	3	3				
N_VLinearSumVectorArray	✓					
N_VScaleVectorArray	✓					
N_VConstVectorArray	✓					
N_VWrmsNormVectorArray	✓					
N_VScaleAddMultiVectorArray	✓					
N_VLinearCombinationVectorArray	✓					

Chapter 9

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.

9.1 The SUNMatrix API

The SUNMATRIX API can be grouped into two sets of functions: the core matrix operations, and utility functions. Section 9.1.1 lists the core operations, while Section 9.1.2 lists the utility functions.

9.1.1 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 9.2.

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`

9.1.2 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`

9.1.3 SUNMatrix return codes

The functions provided to SUNMATRIX modules within the SUNDIALS-provided SUNMATRIX implementations utilize a common set of return codes, shown in Table 9.1. 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 9.1: Description of the `SUNMatrix` return codes

Name	Value	Description
SUNMAT_SUCCESS	0	successful call or converged solve

continued on next page

Table 9.2: 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_SPARSE	Sparse (CSR or CSC) M × N matrix	2
SUNMATRIX_SLUNRLOC	Adapter for the SuperLU_DIST SuperMatrix	3
SUNMATRIX_CUSTOM	User-provided custom matrix	4

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

9.1.4 SUNMatrix identifiers

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 9.2. It is recommended that a user-supplied SUNMATRIX implementation use the SUNMATRIX_CUSTOM identifier.

9.1.5 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 10. More specifically, in Table 9.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 9.3: 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	✓	✓	✓	✓	✓	✓	✓	✓	✓

9.1.6 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 9.1.1 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
```

9.1.7 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 9.1.2.

9.2 SUNMatrix functions used by CVODES

In Table 9.4, we list the matrix functions in the SUNMATRIX module used within the CVODES package. The table also shows, for each function, which of the code modules uses the function. The main CVODES integrator does not call any SUNMATRIX functions directly, so the table columns are specific to the CVLS interface and the CVBANDPRE and CVBBDPRE preconditioner modules. We further note that the CVLS interface only utilizes these routines when supplied with a *matrix-based* linear solver, i.e., the SUNMATRIX object passed to `CVodeSetLinearSolver` was not `NULL`.

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

Table 9.4: List of matrix functions usage by CVODES code modules

	CVLS	CVBANDPRE	CVBBDPRE
SUNMatGetID	✓		
SUNMatClone	✓		
SUNMatDestroy	✓	✓	✓
SUNMatZero	✓	✓	✓
SUNMatCopy	✓	✓	✓
SUNMatScaleAddI	✓	✓	✓
SUNMatSpace	†	†	†

The matrix functions listed in Section 9.1.1 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 9.1.1 that are *not* used by CVODES are: SUNMatScaleAdd and SUNMatMatvec. Therefore a user-supplied SUNMATRIX module for CVODES could omit these functions.

We note that the CVBANDPRE and CVBBDPRE preconditioner modules are hard-coded to use the SUNDIALS-supplied band SUNMATRIX type, so the most useful information above for user-supplied SUNMATRIX implementations is the column relating the CVLS requirements.

9.3 The SUNMatrix_Dense implementation

The dense implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_DENSE, defines the *content* field of SUNMatrix to be the following structure:

```
struct _SUNMatrixContent_Dense {
  sunindextype M;
  sunindextype N;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

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

M - number of rows

N - number of columns

data - pointer to a contiguous block of realtype variables. The elements of the dense matrix are stored columnwise, i.e. the (i,j)-th element of a dense SUNMATRIX A (with $0 \le$ i $<$ M and $0 \le$ j $<$ N) may be accessed via data[j*M+i].

ldata - length of the data array (= M·N).

cols - array of pointers. cols[j] points to the first element of the j-th column of the matrix in the array data. The (i,j)-th element of a dense SUNMATRIX A (with $0 \le$ i $<$ M and $0 \le$ j $<$ N) may be accessed via cols[j][i].

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

9.3.1 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 $\mathtt{M} \times \mathtt{N}$ dense matrix `A` (with $0 \le \mathtt{j} < \mathtt{N}$). 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 $\mathtt{M} - 1$.

  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 $\mathtt{M} \times \mathtt{N}$ dense matrix `A` (with $0 \le \mathtt{i} < \mathtt{M}$ and $0 \le \mathtt{j} < \mathtt{N}$).

  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] )
```

9.3.2 SUNMatrix_Dense functions

The SUNMATRIX_DENSE module defines dense implementations of all matrix operations listed in Section 9.1.1. Their names are obtained from those in Section 9.1.1 by appending the suffix `_Dense` (e.g. `SUNMatCopy_Dense`). All the standard matrix operations listed in Section 9.1.1 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 $\texttt{M} - 1$.

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

Notes

- When looping over the components of a dense `SUNMatrix A`, the most efficient approaches are to:
  - First obtain the component array via `A_data = SM_DATA_D(A)` or `A_data = SUNDenseMatrix_Data(A)` and then access `A_data[i]` within the loop.
  - First obtain the array of column pointers via `A_cols = SM_COLS_D(A)` or `A_cols = SUNDenseMatrix_Cols(A)`, and then access `A_cols[j][i]` within the loop.
  - Within a loop over the columns, access the column pointer via `A_colj = SUNDenseMatrix_Column(A,j)` and then to access the entries within that column using `A_colj[i]` within the loop.

  All three of these are more efficient than using `SM_ELEMENT_D(A,i,j)` within a double loop.

- Within the `SUNMatMatvec_Dense` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

9.3.3 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.

9.4 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 9.1. A more complete description of the parts of this *content* field is given below:

`M` - number of rows

`N` - number of columns (`N` = `M`)

`mu` - upper half-bandwidth, 0 ≤ `mu` < `N`

`ml` - lower half-bandwidth, 0 ≤ `ml` < `N`

`s_mu` - storage upper bandwidth, `mu` ≤ `s_mu` < `N`. The LU decomposition routines in the associated SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as min(`N`-1,`mu`+`ml`) because of partial pivoting. The `s_mu` field holds the upper half-bandwidth allocated for A.

`ldim` - leading dimension (`ldim` ≥ `s_mu`+`ml`+1)

`data` - pointer to a contiguous block of `realtype` variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. `data` is a pointer to `ldata` contiguous locations which hold the elements within the band of A.

`ldata` - length of the data array (= `ldim`·N)

`cols` - array of pointers. `cols[j]` is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from `s_mu`−`mu` (to access the uppermost element within the band in the j-th column) to `s_mu`+`ml` (to access the lowest element within the band in the j-th column). Indices from 0 to `s_mu`−`mu`−1 give access to extra storage elements required by the LU decomposition function. Finally, `cols[j][i-j+s_mu]` is the (i,j)-th element with j−`mu` ≤ i ≤ j+`ml`.

The header file to include when using this module is `sunmatrix/sunmatrix_band.h`. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixband` module library.

9.4.1 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) )
  ```

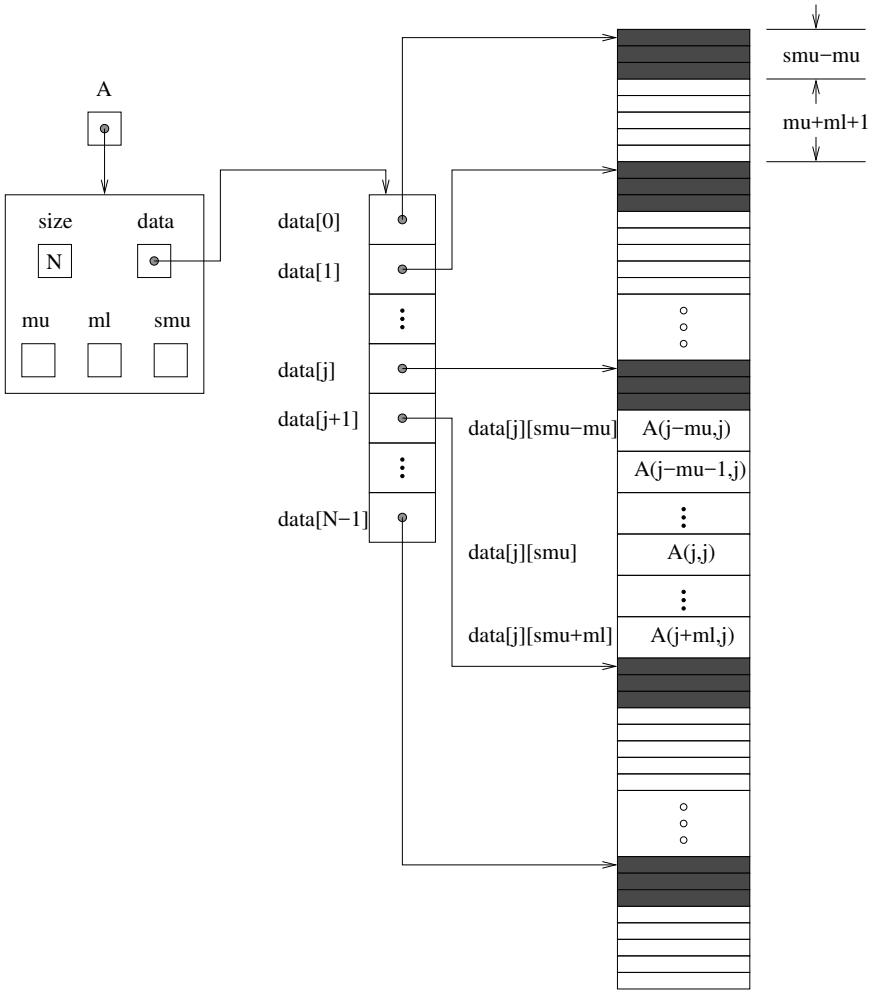

Figure 9.1: Diagram of the storage for the SUNMATRIX_BAND module. Here `A` is an `N` $\times$ `N` band matrix with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of `A` are numbered from 0 to `N` -1 and the (i, j)-th element of `A` is denoted `A(i,j)`. The greyed out areas of the underlying component storage are used by the associated SUNLINSOL_BAND linear solver.

- SM_ROWS_B, SM_COLUMNS_B, SM_UBAND_B, SM_LBAND_B, SM_SUBAND_B, SM_LDIM_B, and SM_LDATA_B

  These macros give individual access to various lengths relevant to the content of a banded SUNMatrix.

  These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_B(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_B(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

  Implementation:

```
#define SM_ROWS_B(A)        ( SM_CONTENT_B(A)->M )
#define SM_COLUMNS_B(A)     ( SM_CONTENT_B(A)->N )
#define SM_UBAND_B(A)       ( SM_CONTENT_B(A)->mu )
#define SM_LBAND_B(A)       ( SM_CONTENT_B(A)->ml )
#define SM_SUBAND_B(A)      ( SM_CONTENT_B(A)->s_mu )
#define SM_LDIM_B(A)        ( SM_CONTENT_B(A)->ldim )
#define SM_LDATA_B(A)       ( SM_CONTENT_B(A)->ldata )
```

- SM_DATA_B and SM_COLS_B

  These macros give access to the `data` and `cols` pointers for the matrix entries.

  The assignment `A_data = SM_DATA_B(A)` sets `A_data` to be a pointer to the first component of the data array for the banded SUNMatrix `A`. The assignment `SM_DATA_B(A) = A_data` sets the data array of `A` to be `A_data` by storing the pointer `A_data`.

  Similarly, the assignment `A_cols = SM_COLS_B(A)` sets `A_cols` to be a pointer to the array of column pointers for the banded SUNMatrix `A`. The assignment `SM_COLS_B(A) = A_cols` sets the column pointer array of `A` to be `A_cols` by storing the pointer `A_cols`.

  Implementation:

```
#define SM_DATA_B(A)        ( SM_CONTENT_B(A)->data )
#define SM_COLS_B(A)        ( SM_CONTENT_B(A)->cols )
```

- SM_COLUMN_B, SM_COLUMN_ELEMENT_B, and SM_ELEMENT_B

  These macros give access to the individual columns and entries of the data array of a banded SUNMatrix.

  The assignments `SM_ELEMENT_B(A,i,j) = a_ij` and `a_ij = SM_ELEMENT_B(A,i,j)` reference the (`i`,`j`)-th element of the `N` × `N` band matrix `A`, where $0 \le$ `i`, `j` $\le$ `N` $- 1$. The location (`i`,`j`) should further satisfy `j`$-$`mu` $\le$ `i` $\le$ `j`$+$`ml`.

  The assignment `col_j = SM_COLUMN_B(A,j)` sets `col_j` to be a pointer to the diagonal element of the `j`-th column of the `N` × `N` band matrix `A`, $0 \le$ `j` $\le$ `N` $- 1$. The type of the expression `SM_COLUMN_B(A,j)` is `realtype *`. The pointer returned by the call `SM_COLUMN_B(A,j)` can be treated as an array which is indexed from $-$`mu` to `ml`.

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

  Implementation:

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

9.4.2 SUNMatrix_Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Section 9.1.1. Their names are obtained from those in Section 9.1.1 by appending the suffix `_Band` (e.g. `SUNMatCopy_Band`). All the standard matrix operations listed in Section 9.1.1 with the suffix `_Band` appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. `FSUNMatCopy_Band`).

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

`SUNBandMatrix`

Prototype `SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu, sunindextype ml)`

Description This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, and the upper and lower half-bandwidths of the matrix, `mu` and `ml`. The stored upper bandwidth is set to `mu+ml` to accommodate subsequent factorization in the SUNLINSOL_BAND and SUNLINSOL_LAPACKBAND modules.

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

`SUNBandMatrixStorage`

Prototype `SUNMatrix SUNBandMatrixStorage(sunindextype N, sunindextype mu, sunindextype ml, sunindextype smu)`

Description This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, the upper and lower half-bandwidths of the matrix, `mu` and `ml`, and the stored upper bandwidth, `smu`. When creating a band `SUNMatrix`, this value should be

- at least min(`N`-1,`mu`+`ml`) if the matrix will be used by the SUNLINSOL_BAND module;
- exactly equal to `mu`+`ml` if the matrix will be used by the SUNLINSOL_LAPACKBAND module;
- at least `mu` if used in some other manner.

Note: it is strongly recommended that users call the default constructor, `SUNBandMatrix`*, in all standard use cases. This advanced constructor is used internally within* SUNDIALS *solvers, and is provided to users who require banded matrices for non-default purposes.*

`SUNBandMatrix_Print`

Prototype `void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile)`

Description This function prints the content of a banded `SUNMatrix` to the output stream specified by `outfile`. Note: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

`SUNBandMatrix_Rows`

Prototype `sunindextype SUNBandMatrix_Rows(SUNMatrix A)`

Description This function returns the number of rows in the banded `SUNMatrix`.

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

`SUNBandMatrix_Columns`

Prototype `sunindextype SUNBandMatrix_Columns(SUNMatrix A)`

Description This function returns the number of columns in the banded `SUNMatrix`.

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

`SUNBandMatrix_LowerBandwidth`

Prototype `sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A)`

Description This function returns the lower half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_UpperBandwidth`

Prototype `sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A)`

Description This function returns the upper half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_StoredUpperBandwidth`

Prototype `sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A)`

Description This function returns the stored upper half-bandwidth of the banded `SUNMatrix`.

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

`SUNBandMatrix_LDim`

Prototype `sunindextype SUNBandMatrix_LDim(SUNMatrix A)`

Description This function returns the length of the leading dimension of the banded `SUNMatrix`.

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

`SUNBandMatrix_Data`

Prototype `realtype* SUNBandMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the banded `SUNMatrix`.

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

`SUNBandMatrix_Cols`

Prototype `realtype** SUNBandMatrix_Cols(SUNMatrix A)`

Description This function returns a pointer to the cols array for the banded `SUNMatrix`.

SUNBandMatrix_Column

Prototype `realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j)`

Description This function returns a pointer to the diagonal entry of the j-th column of the banded `SUNMatrix`. The resulting pointer should be indexed over the range $-$`mu` to `ml`.

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

Notes

- When looping over the components of a banded `SUNMatrix A`, the most efficient approaches are to:
  - First obtain the component array via `A_data = SM_DATA_B(A)` or `A_data = SUNBandMatrix_Data(A)` and then access `A_data[i]` within the loop.
  - First obtain the array of column pointers via `A_cols = SM_COLS_B(A)` or `A_cols = SUNBandMatrix_Cols(A)`, and then access `A_cols[j][i]` within the loop.
  - Within a loop over the columns, access the column pointer via `A_colj = SUNBandMatrix_Column(A,j)` and then to access the entries within that column using `SM_COLUMN_ELEMENT_B(A_colj,i,j)`.

  All three of these are more efficient than using `SM_ELEMENT_B(A,i,j)` within a double loop.

- Within the `SUNMatMatvec_Band` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

9.4.3 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.

9.5 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 9.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

`M` - number of rows

`N` - number of columns

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

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

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

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

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

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

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

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

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

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

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

For example, the 5×4 CSC matrix

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

could be stored in this structure as either

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

or

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

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

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

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

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

9.5.1 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.

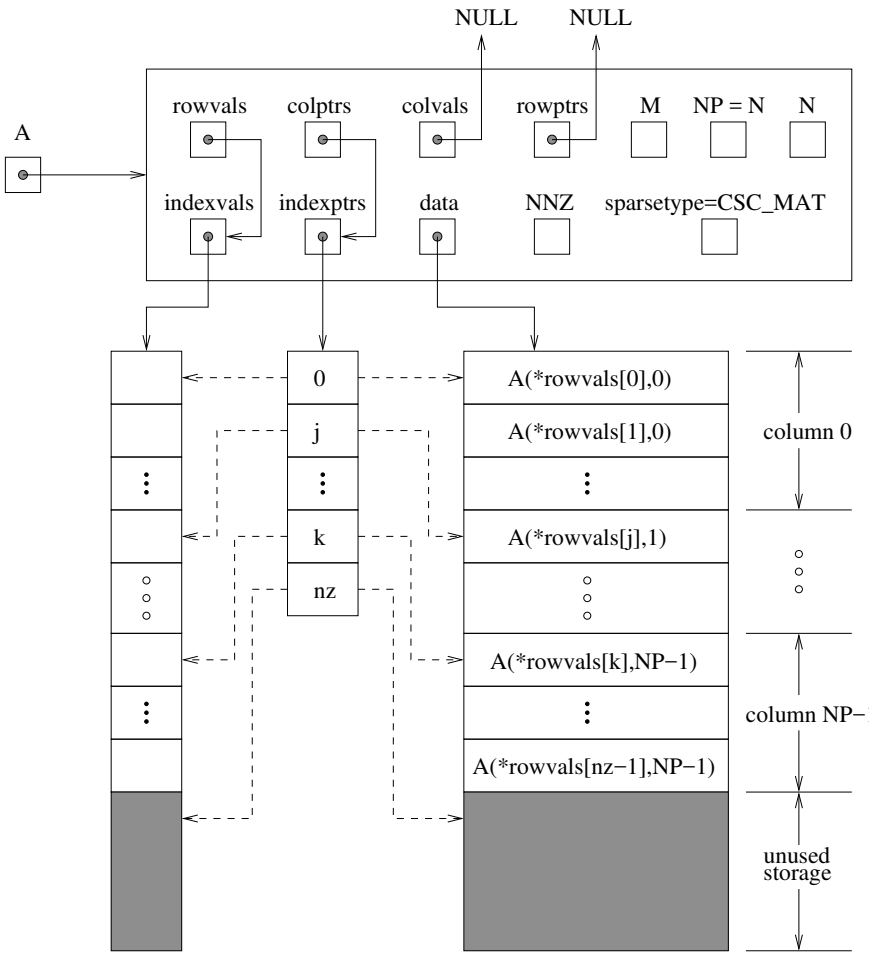

Figure 9.2: Diagram of the storage for a compressed-sparse-column matrix. Here `A` is an $\texttt{M} \times \texttt{N}$ sparse matrix with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to $\texttt{M} - 1$, corresponding to the row index (zero-based) of each nonzero value. The entries in `data` contain the values of the nonzero entries, with the row i, column j entry of `A` (again, zero-based) denoted as `A(i,j)`. The `indexptrs` array contains $\texttt{N}+1$ entries; the first `N` denote the starting index of each column within the `indexvals` and `data` arrays, while the final entry points one past the final nonzero entry. Here, although `NNZ` values are allocated, only `nz` are actually filled in; the greyed-out portions of `data` and `indexvals` indicate extra allocated space.

Implementation:

```
#define SM_CONTENT_S(A)     ( (SUNMatrixContent_Sparse)(A->content) )
```

- SM_ROWS_S, SM_COLUMNS_S, SM_NNZ_S, SM_NP_S, and SM_SPARSETYPE_S

  These macros give individual access to various lengths relevant to the content of a sparse SUNMatrix.

  These may be used either to retrieve or to set these values. For example, the assignment A_rows = SM_ROWS_S(A) sets A_rows to be the number of rows in the matrix A. Similarly, the assignment SM_COLUMNS_S(A) = A_cols sets the number of columns in A to equal A_cols.

  Implementation:

```
#define SM_ROWS_S(A)        ( SM_CONTENT_S(A)->M )
#define SM_COLUMNS_S(A)     ( SM_CONTENT_S(A)->N )
#define SM_NNZ_S(A)         ( SM_CONTENT_S(A)->NNZ )
#define SM_NP_S(A)          ( SM_CONTENT_S(A)->NP )
#define SM_SPARSETYPE_S(A)  ( SM_CONTENT_S(A)->sparsetype )
```

- SM_DATA_S, SM_INDEXVALS_S, and SM_INDEXPTRS_S

  These macros give access to the data and index arrays for the matrix entries.

  The assignment A_data = SM_DATA_S(A) sets A_data to be a pointer to the first component of the data array for the sparse SUNMatrix A. The assignment SM_DATA_S(A) = A_data sets the data array of A to be A_data by storing the pointer A_data.

  Similarly, the assignment A_indexvals = SM_INDEXVALS_S(A) sets A_indexvals to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix A. The assignment A_indexptrs = SM_INDEXPTRS_S(A) sets A_indexptrs to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).

  Implementation:

```
#define SM_DATA_S(A)        ( SM_CONTENT_S(A)->data )
#define SM_INDEXVALS_S(A)   ( SM_CONTENT_S(A)->indexvals )
#define SM_INDEXPTRS_S(A)   ( SM_CONTENT_S(A)->indexptrs )
```

9.5.2 SUNMatrix_Sparse functions

The SUNMATRIX_SPARSE module defines sparse implementations of all matrix operations listed in Section 9.1.1. Their names are obtained from those in Section 9.1.1 by appending the suffix _Sparse (e.g. SUNMatCopy_Sparse). All the standard matrix operations listed in Section 9.1.1 with the suffix _Sparse appended are callable via the FORTRAN 2003 interface by prepending an 'F' (e.g. FSUNMatCopy_Sparse).

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

SUNSparseMatrix

Prototype
```
SUNMatrix SUNSparseMatrix(sunindextype M, sunindextype N,
                          sunindextype NNZ, int sparsetype)
```

Description This function creates and allocates memory for a sparse SUNMatrix. Its arguments are the number of rows and columns of the matrix, M and N, the maximum number of nonzeros to be stored in the matrix, NNZ, and a flag sparsetype indicating whether to use CSR or CSC format (valid arguments are CSR_MAT or CSC_MAT).

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

`SUNSparseFromDenseMatrix`

Prototype `SUNMatrix SUNSparseFromDenseMatrix(SUNMatrix A, realtype droptol, int sparsetype);`

Description This function creates a new sparse matrix from an existing dense matrix by copying all values with magnitude larger than `droptol` into the sparse matrix structure.

Requirements:

- `A` must have type `SUNMATRIX_DENSE`;
- `droptol` must be non-negative;
- `sparsetype` must be either `CSC_MAT` or `CSR_MAT`.

The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

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

`SUNSparseFromBandMatrix`

Prototype `SUNMatrix SUNSparseFromBandMatrix(SUNMatrix A, realtype droptol, int sparsetype);`

Description This function creates a new sparse matrix from an existing band matrix by copying all values with magnitude larger than `droptol` into the sparse matrix structure.

Requirements:

- `A` must have type `SUNMATRIX_BAND`;
- `droptol` must be non-negative;
- `sparsetype` must be either `CSC_MAT` or `CSR_MAT`.

The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

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

`SUNSparseMatrix_Realloc`

Prototype `int SUNSparseMatrix_Realloc(SUNMatrix A)`

Description This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has no wasted space (i.e. the space allocated for nonzero entries equals the actual number of nonzeros, `indexptrs[NP]`). Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse).

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

`SUNSparseMatrix_Reallocate`

Prototype `int SUNSparseMatrix_Reallocate(SUNMatrix A, sunindextype NNZ)`

Description This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has storage for a specified number of nonzeros. Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse or if NNZ is negative).

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

`SUNSparseMatrix_Print`

Prototype `void SUNSparseMatrix_Print(SUNMatrix A, FILE* outfile)`

Description This function prints the content of a sparse `SUNMatrix` to the output stream specified by `outfile`. Note: `stdout` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

`SUNSparseMatrix_Rows`

Prototype `sunindextype SUNSparseMatrix_Rows(SUNMatrix A)`

Description This function returns the number of rows in the sparse `SUNMatrix`.

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

`SUNSparseMatrix_Columns`

Prototype `sunindextype SUNSparseMatrix_Columns(SUNMatrix A)`

Description This function returns the number of columns in the sparse `SUNMatrix`.

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

`SUNSparseMatrix_NNZ`

Prototype `sunindextype SUNSparseMatrix_NNZ(SUNMatrix A)`

Description This function returns the number of entries allocated for nonzero storage for the sparse matrix `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_NNZ` when using the Fortran 2003 interface module.

`SUNSparseMatrix_NP`

Prototype `sunindextype SUNSparseMatrix_NP(SUNMatrix A)`

Description This function returns the number of columns/rows for the sparse `SUNMatrix`, depending on whether the matrix uses CSC/CSR format, respectively. The `indexptrs` array has `NP+1` entries.

F2003 Name This function is callable as `FSUNSparseMatrix_NP` when using the Fortran 2003 interface module.

`SUNSparseMatrix_SparseType`

Prototype `int SUNSparseMatrix_SparseType(SUNMatrix A)`

Description This function returns the storage type (`CSR_MAT` or `CSC_MAT`) for the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_SparseType` when using the Fortran 2003 interface module.

`SUNSparseMatrix_Data`

Prototype `realtype* SUNSparseMatrix_Data(SUNMatrix A)`

Description This function returns a pointer to the data array for the sparse `SUNMatrix`.

F2003 Name This function is callable as `FSUNSparseMatrix_Data` when using the Fortran 2003 interface module.

`SUNSparseMatrix_IndexValues`

Prototype `sunindextype* SUNSparseMatrix_IndexValues(SUNMatrix A)`

Description This function returns a pointer to index value array for the sparse `SUNMatrix`: for CSR format this is the column index for each nonzero entry, for CSC format this is the row index for each nonzero entry.

F2003 Name This function is callable as `FSUNSparseMatrix_IndexValues` when using the Fortran 2003 interface module.

`SUNSparseMatrix_IndexPointers`

Prototype `sunindextype* SUNSparseMatrix_IndexPointers(SUNMatrix A)`

Description This function returns a pointer to the index pointer array for the sparse `SUNMatrix`: for CSR format this is the location of the first entry of each row in the `data` and `indexvalues` arrays, for CSC format this is the location of the first entry of each column.

F2003 Name This function is callable as `FSUNSparseMatrix_IndexPointers` when using the Fortran 2003 interface module.

Within the `SUNMatMatvec_Sparse` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: NVECTOR_SERIAL, NVECTOR_OPENMP, NVECTOR_PTHREADS, and NVECTOR_CUDA when using managed memory. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.

9.5.3 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.

9.6 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 [3, 24, 40, 41]. It is designed to be used with the SUNLINSOL_SUPERLUDIST linear solver discussed in Section 10.10. 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.

9.6.1 SUNMatrix_SLUNRloc functions

The module SUNMATRIX_SLUNRLOC provides the following user-callable routines:

`SUNMatrix_SLUNRloc`

Call `A = SUNMatrix_SLUNRloc(Asuper, grid);`

Description The function `SUNMatrix_SLUNRloc` creates and allocates memory for a SUNMATRIX_SLUNRLOC object.

Arguments `Asuper` (`SuperMatrix*`) a fully-allocated SuperLU_DIST `SuperMatrix` that the SUNMatrix will wrap; must have `Stype = SLU_NR_loc, Dtype = SLU_D, Mtype = SLU_GE` to be compatible

`grid` (`gridinfo_t*`) the initialized SuperLU_DIST 2D process grid structure

Return value a `SUNMatrix` object if `Asuper` is compatible else `NULL`

Notes

`SUNMatrix_SLUNRloc_Print`

Call `SUNMatrix_SLUNRloc_Print(A, fp);`

Description The function `SUNMatrix_SLUNRloc_Print` prints the underlying `SuperMatrix` content.

Arguments `A` (`SUNMatrix`) the matrix to print
`fp` (`FILE`) the file pointer used for printing

Return value `void`

Notes

`SUNMatrix_SLUNRloc_SuperMatrix`

Call `Asuper = SUNMatrix_SLUNRloc_SuperMatrix(A);`

Description The function `SUNMatrix_SLUNRloc_SuperMatrix` provides access to the underlying SuperLU_DIST `SuperMatrix` of `A`.

Arguments `A` (`SUNMatrix`) the matrix to access

Return value `SuperMatrix*`

Notes

`SUNMatrix_SLUNRloc_ProcessGrid`

Call `grid = SUNMatrix_SLUNRloc_ProcessGrid(A);`

Description The function `SUNMatrix_SLUNRloc_ProcessGrid` provides access to the SuperLU_DIST `gridinfo_t` structure associated with `A`.

Arguments `A` (`SUNMatrix`) the matrix to access

Return value `gridinfo_t*`

Notes

`SUNMatrix_SLUNRloc_OwnData`

Call `does_own_data = SUNMatrix_SLUNRloc_OwnData(A);`

Description The function `SUNMatrix_SLUNRloc_OwnData` returns true if the `SUNMatrix` object is responsible for freeing `A_super`, otherwise it returns false.

Arguments `A` (`SUNMatrix`) the matrix to access

Return value `booleantype`

Notes

The SUNMATRIX_SLUNRLOC module defines implementations of all generic `SUNMatrix` operations listed in Section 9.1.1:

- `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.

Chapter 10

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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{10.1}$$

where

$$\begin{aligned} \tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\ \tilde{b} &= S_1 P_1^{-1} b, \\ \tilde{x} &= S_2 P_2 x, \end{aligned} \tag{10.2}$$

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 §10.4.2 for more details). In this case, they instead request that iterative linear solvers stop based on the criteria

$$\left\| P_1^{-1} b - P_1^{-1} A x \right\|_2 < \text{tol}.$$

We note that the corresponding adjustments to tol in this case are non-optimal, in that they cannot balance error between specific entries of the solution x, only the aggregate error in the overall solution vector.

We further note that not all of the SUNDIALS-provided iterative linear solvers support the full range of the above options (e.g., separate left/right preconditioning), and that some of the SUNDIALS packages only utilize a subset of these options. Further details on these exceptions are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS package.

For users interested in providing their own SUNLINSOL module, the following section presents the SUNLINSOL API and its implementation beginning with the definition of SUNLINSOL functions in sections 10.1.1 – 10.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 10.1.4. A table of linear solver return codes is given in section 10.1.5. The `SUNLinearSolver` type and the generic SUNLINSOL module are defined in section 10.1.6. The section 10.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 10.3 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 10.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

10.1 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`.

10.1.1 `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 10.3.1 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 10.1.

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 10.1.

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 10.1.

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`

10.1.2 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 10.1.

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 (10.1)-(10.2). 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 10.1.

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 (10.1)-(10.2), 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 10.1.

F2003 Name `FSUNLinSolSetScalingVectors`

10.1.3 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 10.1.

Notes This function is advisory only, for use in determining a user's total space requirements.

F2003 Name `FSUNLinSolSpace`

10.1.4 Functions provided by SUNDIALS packages

To interface with the SUNLINSOL modules, the SUNDIALS packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic interfaces to the linear systems of equations that result in their solution. The types for functions provided to a SUNLINSOL module are defined in the header file `sundials/sundials_iterative.h`, and are described below.

`ATimesFn`

Definition `typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);`

Purpose These functions compute the action of a matrix on a vector, performing the operation $z = Av$. Memory for `z` should already be allocted prior to calling this function. The vector `v` should be left unchanged.

Arguments `A_data` is a pointer to client data, the same as that supplied to `SUNLinSolSetATimes`.
`v` is the input vector to multiply.
`z` is the output vector computed.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

`PSetupFn`

Definition `typedef int (*PSetupFn)(void *P_data)`

Purpose These functions set up any requisite problem data in preparation for calls to the corresponding `PSolveFn`.

Arguments `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful.

PSolveFn

Definition
```
typedef int (*PSolveFn)(void *P_data, N_Vector r, N_Vector z,
                        realtype tol, int lr)
```

Purpose These functions solve the preconditioner equation $Pz = r$ for the vector z. Memory for `z` should already be allocted prior to calling this function. The parameter `P_data` is a pointer to any information about P which the function needs in order to do its job (set up by the corresponding `PSetupFn`). The parameter `lr` is input, and indicates whether P is to be taken as the left preconditioner or the right preconditioner: `lr` $= 1$ for left and `lr` $= 2$ for right. If preconditioning is on one side only, `lr` can be ignored. If the preconditioner is iterative, then it should strive to solve the preconditioner equation so that

$$\|Pz - r\|_{\text{wrms}} < tol$$

where the weight vector for the WRMS norm may be accessed from the main package memory structure. The vector `r` should not be modified by the `PSolveFn`.

Arguments
- `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.
- `r` is the right-hand side vector for the preconditioner system.
- `z` is the solution vector for the preconditioner system.
- `tol` is the desired tolerance for an iterative preconditioner.
- `lr` is flag indicating whether the routine should perform left (1) or right (2) preconditioning.

Return value This routine should return 0 if successful and a non-zero value if unsuccessful. On a failure, a negative return value indicates an unrecoverable condition, while a positive value indicates a recoverable one, in which the calling routine may reattempt the solution after updating preconditioner data.

10.1.5 `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 10.1. 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 10.1: 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_FAIL_UNREC	-804	an unrecoverable failure occurred in the `ATimes` routine

continued on next page

Name	Value	Description
SUNLS_PSET_FAIL_UNREC	-805	an unrecoverable failure occurred in the Pset routine
SUNLS_PSOLVE_FAIL_UNREC	-806	an unrecoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_UNREC	-807	an unrecoverable failure occurred in an external linear solver package
SUNLS_GS_FAIL	-808	a failure occurred during Gram-Schmidt orthogonalization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
SUNLS_QRSOL_FAIL	-809	a singular R matrix was encountered in a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPFGMR)
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)

10.1.6 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 10.1.1-10.1.3. 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
```

10.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 10.2 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 10.2: 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	✓	✓	✓	✓	✓

10.3 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 10.4 to determine which SUNLINSOL operations are required for this SUNDIALS package.

  Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNLINSOL module (each with different SUNLinearSolver internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free a SUNLinearSolver with the new *content* field and with *ops* pointing to the new linear solver operations.

We note that the function pointers for all unsupported optional routines should be set to NULL in the *ops* structure. This allows the SUNDIALS package that is using the SUNLINSOL object to know that the associated functionality is not supported.

To aid in the creation of custom SUNLINSOL modules the generic SUNLINSOL module provides the utility functions SUNLinSolNewEmpty and SUNLinSolFreeEmpty. When used in custom SUNLINSOL constructors the function SUNLinSolNewEmpty will ease the introduction of any new optional linear solver operations to the SUNLINSOL API by ensuring only required operations need to be set.

SUNLinSolNewEmpty

Call `LS = SUNLinSolNewEmpty();`

Description The function SUNLinSolNewEmpty allocates a new generic SUNLINSOL object and initializes its content pointer and the function pointers in the operations structure to NULL.

Arguments None

Return value This function returns a SUNLinearSolver object. If an error occurs when allocating the object, then this routine will return NULL.

F2003 Name FSUNLinSolNewEmpty

SUNLinSolFreeEmpty

Call `SUNLinSolFreeEmpty(LS);`

Description This routine frees the generic `SUNLinSolFreeEmpty` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `LS` (`SUNLinearSolver`)

Return value None

F2003 Name `FSUNLinSolFreeEmpty`

Additionally, a SUNLINSOL implementation *may* do the following:

- Define and implement additional user-callable "set" routines acting on the `SUNLinearSolver`, e.g., for setting various configuration options to tune the linear solver to a particular problem.
- Provide additional user-callable "get" routines acting on the `SUNLinearSolver` object, e.g., for returning various solve statistics.

10.3.1 Intended use cases

The SUNLINSOL (and SUNMATRIX) APIs are designed to require a minimal set of routines to ease interfacing with custom or third-party linear solver libraries. External solvers provide similar routines with the necessary functionality and thus will require minimal effort to wrap within custom SUNMATRIX and SUNLINSOL implementations. Sections 9.2 and 10.4 include a list of the required set of routines that compatible SUNMATRIX and SUNLINSOL implementations must provide. As SUNDIALS packages utilize generic SUNLINSOL modules allowing for user-supplied `SUNLinearSolver` implementations, there exists a wide range of possible linear solver combinations. Some intended use cases for both the SUNDIALS-provided and user-supplied SUNLINSOL modules are discussd in the following sections.

Direct linear solvers

Direct linear solver modules require a matrix and compute an 'exact' solution to the linear system *defined by the matrix*. Multiple matrix formats and associated direct linear solvers are supplied with SUNDIALS through different SUNMATRIX and SUNLINSOL implementations. SUNDIALS packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations. As a result, each package's linear solver interface recomputes Jacobian information as infrequently as possible.

Alternative matrix storage formats and compatible linear solvers that are not currently provided by, or interfaced with, SUNDIALS can leverage this infrastructure with minimal effort. To do so, a user must implement custom SUNMATRIX and SUNLINSOL wrappers for the desired matrix format and/or linear solver following the APIs described in Chapters 9 and 10. *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 10.4.2 for more details); however, this use case may be non-optimal and cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single problem.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, SUNDIALS a user must implement a custom SUNLINSOL wrapper for the linear solver following the API described in Chapter 10. *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 §4.5.7.2) 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.

10.4 CVODES SUNLinearSolver interface

Table 10.3 below lists the SUNLINSOL module linear solver functions used within the CVLS interface. As with the SUNMATRIX module, we emphasize that the CVODES user does not need to know detailed usage of linear solver functions by the CVODES code modules in order to use CVODES. 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. `SUNLinSolNumIters` is only used to accumulate overall iterative linear solver statistics. If it is not implemented by the SUNLINSOL module, then CVLS will consider all solves as requiring zero iterations.

2. Although CVLS does not call `SUNLinSolLastFlag` directly, this routine is available for users to query linear solver issues directly.

3. Although CVLS 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 CVLS interface, in the case that interested users wish to develop custom SUNLINSOL modules.

Table 10.3: List of linear solver function usage in the CVLS interface

	DIRECT	ITERATIVE	MATRIX_ITERATIVE
SUNLinSolGetType	✓	✓	✓
SUNLinSolSetATimes	†	✓	†
SUNLinSolSetPreconditioner	†	†	†
SUNLinSolSetScalingVectors	†	†	†
SUNLinSolInitialize	✓	✓	✓
SUNLinSolSetup	✓	✓	✓
SUNLinSolSolve	✓	✓	✓
[1]SUNLinSolNumIters		†	†
[2]SUNLinSolLastFlag			
[3]SUNLinSolFree			
SUNLinSolSpace	†	†	†

10.4.1 Lagged matrix information

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_DIRECT` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`, then the SUNLINSOL object solves a linear system *defined* by a SUNMATRIX object. CVLS will update the matrix information infrequently according to the strategies outlined in §2.1. To this end, we differentiate between the *desired* linear system $Mx = b$ with $M = (I - \gamma J)$, and the *actual* linear system

$$\bar{M}\bar{x} = b \quad \Leftrightarrow \quad (I - \bar{\gamma}J)\bar{x} = b.$$

Since CVLS updates the SUNMATRIX object infrequently, it is likely that $\gamma \neq \bar{\gamma}$, and in turn $M \neq \bar{M}$. When using a BDF method, after calling the SUNLINSOL-provided `SUNLinSolSolve` routine, we test whether $\gamma/\bar{\gamma} \neq 1$, and if this is the case we scale the solution $\bar{x}$ to correct the linear system solution x via

$$x = \frac{2}{1 + \gamma/\bar{\gamma}}\bar{x}. \tag{10.3}$$

The motivation for this selection of the scaling factor $c = 2/(1 + \gamma/\bar{\gamma})$ is discussed in detail in [8, 29]. 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.

10.4.2 Iterative linear solver tolerance

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE` then CVLS 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 CVLS 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 CVODE 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 (10.1)-(10.2)):

$$\begin{aligned}
& \left\| \tilde{b} - \tilde{A}\tilde{x} \right\|_2 < \text{tol} \\
\Leftrightarrow \quad & \left\| SP_1^{-1}b - SP_1^{-1}Ax \right\|_2 < \text{tol} \\
\Leftrightarrow \quad & \sum_{i=0}^{n-1} \left[W_i \left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2 \\
\Leftrightarrow \quad & W_{mean}^2 \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2 \\
\Leftrightarrow \quad & \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \left(\frac{\text{tol}}{W_{mean}} \right)^2 \\
\Leftrightarrow \quad & \left\| P_1^{-1}(b - Ax) \right\|_2 < \frac{\text{tol}}{W_{mean}}
\end{aligned}$$

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2 / \sqrt{n}$$

is computed and the scaled tolerance `delta`$= \text{tol}/W_{mean}$ is supplied to the SUNLINSOL object.

10.5 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.

10.5.1 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).

10.5.2 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 10.1.1 – 10.1.3:

- `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.

10.5.3 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.

10.5.4 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.

10.6 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.

10.6.1 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`.

10.6.2 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 10.1.1 – 10.1.3:

- `SUNLinSolGetType_Band`
- `SUNLinSolInitialize_Band` – this does nothing, since all consistency checks are performed at solver creation.

- SUNLinSolSetup_Band – this performs the LU factorization.
- SUNLinSolSolve_Band – this uses the LU factors and pivots array to perform the solve.
- SUNLinSolLastFlag_Band
- SUNLinSolSpace_Band – this only returns information for the storage *within* the solver object, i.e. storage for N, last_flag, and pivots.
- SUNLinSolFree_Band

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

10.6.3 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.

10.6.4 SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Band {
  sunindextype N;
  sunindextype *pivots;
  sunindextype last_flag;
};
```

These entries of the *content* field contain the following information:

`N` - size of the linear system,

`pivots` - index array for partial pivoting in LU factorization,

`last_flag` - last error return flag from internal function evaluations.

10.7 The SUNLinearSolver_LapackDense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems with LAPACK. The SUNLINSOL_LAPACKDENSE module is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKDENSE module, include the header file `sunlinsol/sunlinsol_lapackdense.h`. The installed module library to link to is `libsundials_sunlinsollapackdense.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_LAPACKDENSE module is a SUNLINSOL wrapper for the LAPACK dense matrix factorization and solve routines, `*GETRF` and `*GETRS`, where `*` is either `D` or `S`, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKDENSE module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKDENSE module also cannot be compiled when using 64-bit integers for the `sunindextype`.

10.7.1 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).

10.7.2 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 10.1.1 – 10.1.3:

- `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`

10.7.3 SUNLinearSolver_LapackDense Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKDENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNLAPACKDENSEINIT`

Call `FSUNLAPACKDENSEINIT(code, ier)`

Description The function `FSUNLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based dense `SUNLinearSolver` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKDENSE module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSLAPACKDENSEINIT`

Call `FSUNMASSLAPACKDENSEINIT(ier)`

Description The function `FSUNMASSLAPACKDENSEINIT` can be called for Fortran programs to create a LAPACK-based, dense `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

10.7.4 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.

10.8 The SUNLinearSolver_LapackBand implementation

This section describes the SUNLINSOL implementation for solving banded linear systems with LAPACK. The SUNLINSOL_LAPACKBAND module is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_LAPACKBAND module, include the header file `sunlinsol/sunlinsol_lapackband.h`. The installed module library to link to is `libsundials_sunlinsollapackband.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_LAPACKBAND module is a SUNLINSOL wrapper for the LAPACK band matrix factorization and solve routines, *GBTRF and *GBTRS, where * is either D or S, depending on whether SUNDIALS was configured to have realtype set to double or single, respectively (see Section 4.2). In order to use the SUNLINSOL_LAPACKBAND module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using extended precision for realtype. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKBAND module also cannot be compiled when using 64-bit integers for the sunindextype.

10.8.1 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.

10.8.2 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 10.1.1 – 10.1.3:

- `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`

10.8.3 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.

10.8.4 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.

10.9 The SUNLinearSolver_KLU implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with KLU. The SUNLINSOL_KLU module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

The header file to include when using this module is `sunlinsol/sunlinsol_klu.h`. The installed module library to link to is `libsundials_sunlinsolklu.`*`lib`* where *`.lib`* is typically `.so` for shared libraries and `.a` for static libraries.

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 17]. In order to use the SUNLINSOL_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to either `extended` or `single` (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available `sunindextype` options.

10.9.1 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.

10.9.2 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 10.1.1 – 10.1.3:

- `SUNLinSolGetType_KLU`
- `SUNLinSolInitialize_KLU` – this sets the `first_factorize` flag to 1, forcing both symbolic and numerical factorizations on the subsequent "setup" call.
- `SUNLinSolSetup_KLU` – this performs either a *LU* factorization or refactorization of the input matrix.
- `SUNLinSolSolve_KLU` – this calls the appropriate KLU solve routine to utilize the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_KLU`
- `SUNLinSolSpace_KLU` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the KLU documentation.

- SUNLinSolFree_KLU

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_KLU module also defines the following additional user-callable functions.

SUNLinSol_KLUReInit

Call `retval = SUNLinSol_KLUReInit(LS, A, nnz, reinit_type);`

Description The function `SUNLinSol_KLUReInit` reinitializes memory and flags for a new factorization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed or if the structure of the linear system has changed which would require a new symbolic (and numeric factorization).

Arguments

`LS`	(`SUNLinearSolver`) a template for cloning vectors needed within the solver
`A`	(`SUNMatrix`) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver
`nnz`	(`sunindextype`) the new number of nonzeros in the matrix
`reinit_type`	(`int`) flag governing the level of reinitialization. The allowed values are:

- `SUNKLU_REINIT_FULL` – The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.
- `SUNKLU_REINIT_PARTIAL` – Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the sparse matrix provided to the original constructor routine (or the previous `SUNLinSol_KLUReInit` call).

Return value The return values from this function are `SUNLS_MEM_NULL` (either `S` or `A` are `NULL`), `SUNLS_ILL_INPUT` (`A` does not have type `SUNMATRIX_SPARSE` or `reinit_type` is invalid), `SUNLS_MEM_FAIL` (reallocation of the sparse matrix failed) or `SUNLS_SUCCESS`.

Notes This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

This routine assumes no other changes to solver use are necessary.

Deprecated Name For backward compatibility, the wrapper function `SUNKLUReInit` with idential input and output arguments is also provided.

F2003 Name `FSUNLinSol_KLUReInit`

SUNLinSol_KLUSetOrdering

Call `retval = SUNLinSol_KLUSetOrdering(LS, ordering);`

Description This function sets the ordering used by KLU for reducing fill in the linear solve.

Arguments

`LS`	(`SUNLinearSolver`) the SUNLINSOL_KLU object
`ordering`	(`int`) flag indicating the reordering algorithm to use, the options are:

0 AMD,

1 COLAMD, and
2 the natural ordering.

The default is 1 for COLAMD.

Return value The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid ordering choice), or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNKLUSetOrdering` with idential input and output arguments is also provided.

F2003 Name `FSUNLinSol_KLUSetOrdering`

`SUNLinSol_KLUGetSymbolic`

Call `symbolic = SUNLinSol_KLUGetSymbolic(LS);`

Description This function returns a pointer to the KLU symbolic factorization stored in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_symbolic`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_symbolic` is mapped to the KLU type `klu_symbolic`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`) this is mapped to the KLU type `klu_l_symbolic`.

`SUNLinSol_KLUGetNumeric`

Call `numeric = SUNLinSol_KLUGetNumeric(LS);`

Description This function returns a pointer to the KLU numeric factorization stored in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_numeric`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_numeric` is mapped to the KLU type `klu_numeric`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`), this is mapped to the KLU type `klu_l_numeric`.

`SUNLinSol_KLUGetCommon`

Call `common = SUNLinSol_KLUGetCommon(LS);`

Description This function returns a pointer to the KLU common structure stored within in the SUNLINSOL_KLU `content` structure.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_KLU object

Return value The return type from this function is `sun_klu_common`.

Notes When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), `sun_klu_common` is mapped to the KLU type `klu_common`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`), this is mapped to the KLU type `klu_l_common`.

10.9.3 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.

10.9.4 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).

10.10 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.

10.10.1 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 [3, 24, 40, 41]. The package uses a SPMD parallel programming model and multithreading to enhance efficiency in distributed-memory parallel environments with multicore nodes and possibly GPU accelerators. It uses MPI for communication, OpenMP for threading, and CUDA for GPU support. In order to use the SUNLINSOL_SUPERLUDIST interface to SuperLU_DIST, it is assumed that SuperLU_DIST has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SuperLU_DIST (see Appendix A for details). Additionally, the adapter only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to use single or extended precision. Moreover, since the SuperLU_DIST library may be installed to support either 32-bit or

64-bit integers, it is assumed that the SuperLU_DIST library is installed using the same integer size as SUNDIALS.

The SuperLU_DIST library provides many options to control how a linear system will be solved. These options may be set by a user on an instance of the `superlu_dist_options_t` struct, and then it may be provided as an argument to the SUNLINSOL_SUPERLUDIST constructor. The SUNLINSOL_SUPERLUDIST module will respect all options set except for `Fact` – this option is necessarily modified by the SUNLINSOL_SUPERLUDIST module in the setup and solve routines.

Since the linear systems that arise within the context of SUNDIALS calculations will typically have identical sparsity patterns, the SUNLINSOL_SUPERLUDIST module is constructed to perform the following operations:

- The first time that the "setup" routine is called, it sets the SuperLU_DIST option `Fact` to `DOFACT` so that a subsequent call to the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to solve the system.

- On subsequent calls to the "setup" routine, it sets the SuperLU_DIST option `Fact` to `SamePattern` so that a subsequent call to "solve" will perform factorization assuming the same sparsity pattern as prior, i.e. it will reuse the column permutation vector.

- If "setup" is called prior to the "solve" routine, then the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to the sparse triangular solves, and, potentially, iterative refinement. If "setup" is not called prior, "solve" will skip to the triangular solve step. We note that in this solve SuperLU_DIST operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

10.10.2 SUNLinearSolver_SuperLUDIST functions

The SUNLINSOL_SUPERLUDIST module defines implementations of all "direct" linear solver operations listed in Sections 10.1.1-10.1.3:

- `SUNLinSolGetType_SuperLUDIST`

- `SUNLinSolInitialize_SuperLUDIST` – this sets the `first_factorize` flag to 1 and resets the internal SuperLU_DIST statistics variables.

- `SUNLinSolSetup_SuperLUDIST` – this sets the appropriate SuperLU_DIST options so that a subsequent solve will perform a symbolic and numerical factorization before proceeding with the triangular solves

- `SUNLinSolSolve_SuperLUDIST` – this calls the SuperLU_DIST solve routine to perform factorization (if the setup routine was called prior) and then use the *LU* factors to solve the linear system.

- `SUNLinSolLastFlag_SuperLUDIST`

- `SUNLinSolSpace_SuperLUDIST` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SuperLU_DIST documentation.

- `SUNLinSolFree_SuperLUDIST`

In addition, the module SUNLINSOL_SUPERLUDIST provides the following user-callable routines:

`SUNLinSol_SuperLUDIST`

Call `LS = SUNLinSol_SuperLUDIST(y, A, grid, lu, scaleperm, solve, stat, options);`

Description The function `SUNLinSol_SuperLUDIST` creates and allocates memory for a SUNLINSOL_SUPERLUDIST object.

Arguments
- `y` (`N_Vector`) a template for cloning vectors needed within the solver
- `A` (`SUNMatrix`) a SUNMATRIX_SLUNRLOC matrix template for cloning matrices needed within the solver
- `grid` (`gridinfo_t*`)
- `lu` (`LUstruct_t*`)
- `scaleperm` (`ScalePermstruct_t*`)
- `solve` (`SOLVEstruct_t*`)
- `stat` (`SuperLUStat_t*`)
- `options` (`superlu_dist_options_t*`)

Return value This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.

Notes This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SuperLU_DIST library.

This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX_SLUNRLOC matrix type and the NVECTOR_SERIAL, NVECTOR_PARALLEL, NVECTOR_PARHYP, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

The `grid`, `lu`, `scaleperm`, `solve`, and `options` arguments are not checked and are passed directly to SuperLU_DIST routines.

Some struct members of the `options` argument are modified internally by the SUNLINSOL_SUPERLUDIST solver. Specifically the member `Fact`, is modified in the setup and solve routines.

`SUNLinSol_SuperLUDIST_GetBerr`

Call `realtype berr = SUNLinSol_SuperLUDIST_GetBerr(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetBerr` returns the componentwise relative backward error of the computed solution.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `realtype`

Notes

`SUNLinSol_SuperLUDIST_GetGridinfo`

Call `gridinfo_t *grid = SUNLinSol_SuperLUDIST_GetGridinfo(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetGridinfo` returns the SuperLU_DIST structure that contains the 2D process grid.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `gridinfo_t*`

Notes

`SUNLinSol_SuperLUDIST_GetLUstruct`

Call `LUstruct_t *lu = SUNLinSol_SuperLUDIST_GetLUstruct(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetLUstruct` returns the SuperLU_DIST structure that contains the distributed L and U factors.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `LUstruct_t*`

Notes

`SUNLinSol_SuperLUDIST_GetSuperLUOptions`

Call `superlu_dist_options_t *opts = SUNLinSol_SuperLUDIST_GetSuperLUOptions(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetSuperLUOptions` returns the SuperLU_DIST structure that contains the options which control how the linear system is factorized and solved.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `superlu_dist_options_t*`

Notes

`SUNLinSol_SuperLUDIST_GetScalePermstruct`

Call `ScalePermstruct_t *sp = SUNLinSol_SuperLUDIST_GetScalePermstruct(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetScalePermstruct` returns the SuperLU_DIST structure that contains the vectors that describe the transformations done to the matrix, A.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `ScalePermstruct_t*`

Notes

`SUNLinSol_SuperLUDIST_GetSOLVEstruct`

Call `SOLVEstruct_t *solve = SUNLinSol_SuperLUDIST_GetSOLVEstruct(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetSOLVEstruct` returns the SuperLU_DIST structure that contains information for communication during the solution phase.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `SOLVEstruct_t*`

Notes

`SUNLinSol_SuperLUDIST_GetSuperLUStat`

Call `SuperLUStat_t *stat = SUNLinSol_SuperLUDIST_GetSuperLUStat(LS);`

Description The function `SUNLinSol_SuperLUDIST_GetSuperLUStat` returns the SuperLU_DIST structure that stores information about runtime and flop count.

Arguments `LS` (`SUNLinearSolver`) the SUNLINSOL_SUPERLUDIST object

Return value `SuperLUStat_t*`

Notes

10.10.3 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;
  LUstruct_t              *lu;
  superlu_dist_options_t  *options;
  ScalePermstruct_t       *scaleperm;
  SOLVEstruct_t           *solve;
  SuperLUStat_t           *stat;
  sunindextype            N;
};
```

These entries of the *content* field contain the following information:

first_factorize - flag indicating whether the factorization has ever been performed,

last_flag - last error return flag from calls to internal routines,

berr - the componentwise relative backward error of the computed solution,

grid - pointer to the SuperLU_DIST structure that stores the 2D process grid,

lu - pointer to the SuperLU_DIST structure that stores the distributed L and U factors,

options - pointer to SuperLU_DIST options structure,

scaleperm - pointer to the SuperLU_DIST structure that stores vectors describing the 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

10.11 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 [4, 39, 19]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step. In order to use the SUNLINSOL_SUPERLUMT interface to SUPERLUMT, it is assumed that SUPERLUMT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SUPERLUMT

(see Appendix A for details). Additionally, this wrapper only supports single- and double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have `realtype` set to `extended` (see Section 4.2). Moreover, since the SUPERLUMT library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SUPERLUMT library is installed using the same integer precision as the SUNDIALS `sunindextype` option.

10.11.1 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.

10.11.2 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 10.1.1 – 10.1.3:

- `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.

10.11.3 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.

10.11.4 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.

10.12 The SUNLinearSolver_cuSolverSp_batchQR implementation

The `SUNLinearSolver_cuSolverSp_batchQR` implementation of the SUNLINSOL API is designed to be used with the SUNMATRIX_SPARSE matrix type, and the NVECTOR_CUDA vector type *with managed memory*. 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.

10.12.1 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 [2]. The module is designed for solving block diagonal linear systems of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_1} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_n} \end{bmatrix}$$

where all block matrices $\mathbf{A_j}$ share the same sparsisty pattern. The matrix must be in the CSR storage format. For further details about the method itself, review the NVIDIA documentation.

10.12.2 SUNLinearSolver_cuSolverSp_batchQR functions

The SUNLinearSolver_cuSolverSp_batchQR module defines implementations of all "direct" linear solver operations listed in Sections 10.1.1-10.1.3:

- 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, nsubsys, subsys_size, subsys_nnz);`

Description The function SUNLinSol_cuSolverSp_batchQR creates and allocates memory for a SUNLINSOL object.

Arguments

`y`	(N_Vector) a NVECTOR_CUDA vector for checking compatibility with the solver
`A`	(SUNMatrix) a SUNMATRIX_SPARSE matrix for checking compatibility with the solver
`nsubsys`	(int) the number of subsystems, i.e., the number of blocks in the matrix
`subsys_size`	(int) the number of rows/columns in a block
`subsys_nnz`	(int) the number of nonzeros in a block

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 SUNMATRIX_SPARSE matrix type and the NVECTOR_CUDA vector type. Since the SUNMATRIX_SPARSE matrix type is only compatible with the NVECTOR_CUDA when using

managed memory, the restriction is also in place for the linear solver. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

`SUNLinSol_cuSolverSp_batchQR_GetDescription`

Call	`SUNLinSol_cuSolverSp_batchQR_GetDescription(LS, &desc);`	
Description	The function `SUNLinSol_cuSolverSp_batchQR_GetDescription` accesses the string description of the object (empty by default).	
Arguments	`LS`	(`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
	`desc`	(`char **`) the string description of the linear solver
Return value	None	

`SUNLinSol_cuSolverSp_batchQR_SetDescription`

Call	`SUNLinSol_cuSolverSp_batchQR_SetDescription(LS, desc);`	
Description	The function `SUNLinSol_cuSolverSp_batchQR_SetDescription` sets the string description of the object (empty by default).	
Arguments	`LS`	(`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
	`desc`	(`const char *`) the string description of the linear solver
Return value	None	

10.12.3 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                nsubsys;            /* number of subsystems                                */
  int                subsys_size;        /* size of each subsystem                              */
  int                subsys_nnz;         /* number of nonzeros per subsystem                    */
  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                                  */
  cusparseMatDescr_t system_description; /* matrix description                                  */
  realtype*          d_values;           /* device array of matrix A values                     */
  int*               d_rowptr;           /* device array of rowptrs for a subsystem             */
  int*               d_colind;           /* device array of column indices for a subsystem      */
  csrqrInfo_t        info;               /* opaque cusolver data structure                      */
  void*              workspace;          /* memory block used by cusolver                       */
  const char*        desc;               /* description of this linear solver                   */
};
```

10.13 The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [48]) 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.

10.13.1 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.

10.13.2 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 10.1.1 – 10.1.3:

- `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`

10.13.3 SUNLinearSolver_SPGMR Fortran interfaces

The SUNLINSOL_SPGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_spgmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPGMR` is interfaced as `FSUNLinSol_SPGMR`.

The FORTRAN 2003 SUNLINSOL_SPGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_spgmr_mod`, and linking to the library `libsundials_fsunlinsolspgmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_spgmr_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolspgmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPGMRINIT`

Call `FSUNSPGMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPGMRINIT`

Call `FSUNMASSSPGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPGMR object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPGMR`.

The `SUNLinSol_SPGMRSetPrecType`, `SUNLinSol_SPGMRSetGSType` and `SUNLinSol_SPGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPGMRSETGSTYPE`

Call `FSUNSPGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

`FSUNMASSSPGMRSETGSTYPE`

Call `FSUNMASSSPGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetGSType` for complete further documentation of this routine.

`FSUNSPGMRSETPRECTYPE`

Call `FSUNSPGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPGMRSETPRECTYPE`

Call `FSUNMASSSPGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetPrecType` for complete further documentation of this routine.

`FSUNSPGMRSETMAXRS`

Call `FSUNSPGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

FSUNMASSSPGMRSETMAXRS

Call `FSUNMASSSPGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPGMRSetMaxRestarts` for complete further documentation of this routine.

10.13.4 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;
};
```

These entries of the *content* field contain the following information:

`maxl` - number of GMRES basis vectors to use (default is 5),

`pretype` - flag for type of preconditioning to employ (default is none),

`gstype` - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

`max_restarts` - number of GMRES restarts to allow (default is 0),

`numiters` - number of iterations from the most-recent solve,

`resnorm` - final linear residual norm from the most-recent solve,

`last_flag` - last error return flag from an internal function,

`ATimes` - function pointer to perform Av product,

`ATData` - pointer to structure for `ATimes`,

`Psetup` - function pointer to preconditioner setup routine,

`Psolve` - function pointer to preconditioner solve routine,

`PData` - pointer to structure for `Psetup` and `Psolve`,

`s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

`V` - the array of Krylov basis vectors $v_1, \ldots, v_{\texttt{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

`Hes` - the $(\texttt{maxl}+1) \times \texttt{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`.,

`givens` - a length `2*maxl` array which represents the Givens rotation matrices that arise in the GMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where

$$F_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & -s_i & & & \\ & & & s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix},$$

are represented in the `givens` vector as `givens[0]` = c_0, `givens[1]` = s_0, `givens[2]` = c_1, `givens[3]` = s_1, ...`givens[2j]` = c_j, `givens[2j+1]` = s_j.,

`xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

`yg` - a length `(maxl+1)` array of `realtype` values used to hold "short" vectors (e.g. y and g),

`vtemp` - temporary vector storage.

10.14 The SUNLinearSolver_SPFGMR implementation

This section describes the SUNLINSOL implementation of the SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [47]) 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.

10.14.1 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.

10.14.2 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 10.1.1 – 10.1.3:

- `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`

10.14.3 SUNLinearSolver_SPFGMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_spfgmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPFGMR` is interfaced as `FSUNLinSol_SPFGMR`.

The FORTRAN 2003 SUNLINSOL_SPFGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_spfgmr_mod`, and linking to the library `libsundials_fsunlinsolspfgmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_spfgmr_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolspfgmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPFGMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPFGMRINIT`

Call	`FSUNSPFGMRINIT(code, pretype, maxl, ier)`
Description	The function `FSUNSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object.
Arguments	`code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE). `pretype` (`int*`) flag indicating desired preconditioning type `maxl` (`int*`) flag indicating Krylov subspace size
Return value	`ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.
Notes	This routine must be called *after* the NVECTOR object has been initialized. Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPFGMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPFGMRINIT`

Call `FSUNMASSSPFGMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPFGMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPFGMR object for mass matrix linear systems.

Arguments `pretype` (`int*`) flag indicating desired preconditioning type
`maxl` (`int*`) flag indicating Krylov subspace size

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPFGMR`.

The `SUNLinSol_SPFGMRSetPrecType`, `SUNLinSol_SPFGMRSetGSType` and `SUNLinSol_SPFGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPFGMRSETGSTYPE`

Call `FSUNSPFGMRSETGSTYPE(code, gstype, ier)`

Description The function `FSUNSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`gstype` (`int*`) flag indicating the desired orthogonalization algorithm.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETGSTYPE`

Call `FSUNMASSSPFGMRSETGSTYPE(gstype, ier)`

Description The function `FSUNMASSSPFGMRSETGSTYPE` can be called for Fortran programs to change the Gram-Schmidt orthogonaliation algorithm for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETGSTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetGSType` for complete further documentation of this routine.

`FSUNSPFGMRSETPRECTYPE`

Call `FSUNSPFGMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
`pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETPRECTYPE`

Call `FSUNMASSSPFGMRSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSSPFGMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetPrecType` for complete further documentation of this routine.

`FSUNSPFGMRSETMAXRS`

Call `FSUNSPFGMRSETMAXRS(code, maxrs, ier)`

Description The function `FSUNSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxrs` (`int*`) maximum allowed number of restarts.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

`FSUNMASSSPFGMRSETMAXRS`

Call `FSUNMASSSPFGMRSETMAXRS(maxrs, ier)`

Description The function `FSUNMASSSPFGMRSETMAXRS` can be called for Fortran programs to change the maximum number of restarts allowed for SPFGMR for mass matrix linear systems.

Arguments The arguments are identical to `FSUNSPFGMRSETMAXRS` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_SPFGMRSetMaxRestarts` for complete further documentation of this routine.

10.14.4 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;
};
```

These entries of the *content* field contain the following information:

`maxl` - number of FGMRES basis vectors to use (default is 5),

`pretype` - flag for type of preconditioning to employ (default is none),

`gstype` - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

`max_restarts` - number of FGMRES restarts to allow (default is 0),

`numiters` - number of iterations from the most-recent solve,

`resnorm` - final linear residual norm from the most-recent solve,

`last_flag` - last error return flag from an internal function,

`ATimes` - function pointer to perform Av product,

`ATData` - pointer to structure for `ATimes`,

`Psetup` - function pointer to preconditioner setup routine,

`Psolve` - function pointer to preconditioner solve routine,

`PData` - pointer to structure for `Psetup` and `Psolve`,

`s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

`V` - the array of Krylov basis vectors $v_1, \ldots, v_{\texttt{maxl}+1}$, stored in `V[0]`, ..., `V[maxl]`. Each v_i is a vector of type NVECTOR.,

`Z` - the array of preconditioned Krylov basis vectors $z_1, \ldots, z_{\texttt{maxl}+1}$, stored in `Z[0]`, ..., `Z[maxl]`. Each z_i is a vector of type NVECTOR.,

`Hes` - the (`maxl` + 1) × `maxl` Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`.,

`givens` - a length `2*maxl` array which represents the Givens rotation matrices that arise in the FGMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where

$$F_i = \begin{bmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & c_i & -s_i & & & \\ & & & s_i & c_i & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix},$$

are represented in the `givens` vector as `givens[0]` = c_0, `givens[1]` = s_0, `givens[2]` = c_1, `givens[3]` = s_1, ... `givens[2j]` = c_j, `givens[2j+1]` = s_j.,

`xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

`yg` - a length `(maxl+1)` array of `realtype` values used to hold "short" vectors (e.g. y and g),

`vtemp` - temporary vector storage.

10.15 The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [51]) 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.

10.15.1 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.

10.15.2 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 10.1.1 – 10.1.3:

- `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`

10.15.3 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.

10.15.4 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;
};
```

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.

10.16 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [23]) iterative linear solver. The SUNLINSOL_SPTFQMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, SPTFQMR requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_SPTFQMR module, include the header file `sunlinsol/sunlinsol_sptfqmr.h`. We note that the SUNLINSOL_SPTFQMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolsptfqmr` module library.

10.16.1 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.

10.16.2 SUNLinearSolver_SPTFQMR functions

The SUNLINSOL_SPTFQMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPTFQMR

Call	`LS = SUNLinSol_SPTFQMR(y, pretype, maxl);`
Description	The function SUNLinSol_SPTFQMR creates and allocates memory for a SPTFQMR SUNLinearSolver object.
Arguments	`y` (N_Vector) a template for cloning vectors needed within the solver `pretype` (int) flag indicating the desired type of preconditioning, allowed values are: • PREC_NONE (0) • PREC_LEFT (1) • PREC_RIGHT (2) • PREC_BOTH (3) Any other integer input will result in the default (no preconditioning). `maxl` (int) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).
Return value	This returns a SUNLinearSolver object. If either y is incompatible then this routine will return NULL.
Notes	This routine will perform consistency checks to ensure that it is called with a consistent NVECTOR implementation (i.e. that it supplies the requisite vector operations). If y is incompatible, then this routine will return NULL. We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLINSOL_SPTFQMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.
Deprecated Name	For backward compatibility, the wrapper function SUNSPTFQMR with idential input and output arguments is also provided.
F2003 Name	FSUNLinSol_SPTFQMR

The SUNLINSOL_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in Sections 10.1.1 – 10.1.3:

- SUNLinSolGetType_SPTFQMR
- SUNLinSolInitialize_SPTFQMR
- SUNLinSolSetATimes_SPTFQMR
- SUNLinSolSetPreconditioner_SPTFQMR
- SUNLinSolSetScalingVectors_SPTFQMR
- SUNLinSolSetup_SPTFQMR
- SUNLinSolSolve_SPTFQMR
- SUNLinSolNumIters_SPTFQMR
- SUNLinSolResNorm_SPTFQMR
- SUNLinSolResid_SPTFQMR

- SUNLinSolLastFlag_SPTFQMR
- SUNLinSolSpace_SPTFQMR
- SUNLinSolFree_SPTFQMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an 'F' to the function name.

The SUNLINSOL_SPTFQMR module also defines the following additional user-callable functions.

SUNLinSol_SPTFQMRSetPrecType

Call	`retval = SUNLinSol_SPTFQMRSetPrecType(LS, pretype);`
Description	The function `SUNLinSol_SPTFQMRSetPrecType` updates the type of preconditioning to use in the SUNLINSOL_SPTFQMR object.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPTFQMR object to update `pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPTFQMR`.
Return value	This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
Deprecated Name	For backward compatibility, the wrapper function `SUNSPTFQMRSetPrecType` with idential input and output arguments is also provided.
F2003 Name	`FSUNLinSol_SPTFQMRSetPrecType`

SUNLinSol_SPTFQMRSetMaxl

Call	`retval = SUNLinSol_SPTFQMRSetMaxl(LS, maxl);`
Description	The function `SUNLinSol_SPTFQMRSetMaxl` updates the number of linear solver iterations to allow.
Arguments	`LS` (`SUNLinearSolver`) the SUNLINSOL_SPTFQMR object to update `maxl` (`int`) flag indicating the number of iterations to allow; values ≤ 0 will result in the default value (5)
Return value	This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.
F2003 Name	`FSUNLinSol_SPTFQMRSetMaxl`

SUNSPTFQMRSetMaxl

10.16.3 SUNLinearSolver_SPTFQMR Fortran interfaces

The SUNLINSOL_SPFGMR module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_sptfqmr_mod` FORTRAN module defines interfaces to all SUNLINSOL_SPFGMR C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_SPTFQMR` is interfaced as `FSUNLinSol_SPTFQMR`.

The FORTRAN 2003 SUNLINSOL_SPFGMR interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_sptfqmr_mod`, and linking to the library `libsundials_fsunlinsolsptfqmr_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_sptfqmr_mod.mod` are installed see Appendix A. We note that the module is accessible

from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolsptfqmr_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_SPTFQMR module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

`FSUNSPTFQMRINIT`

Call `FSUNSPTFQMRINIT(code, pretype, maxl, ier)`

Description The function `FSUNSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_SPTFQMR module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

`FSUNMASSSPTFQMRINIT`

Call `FSUNMASSSPTFQMRINIT(pretype, maxl, ier)`

Description The function `FSUNMASSSPTFQMRINIT` can be called for Fortran programs to create a SUNLINSOL_SPTFQMR object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_SPTFQMR`.

The `SUNLinSol_SPTFQMRSetPrecType` and `SUNLinSol_SPTFQMRSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

`FSUNSPTFQMRSETPRECTYPE`

Call `FSUNSPTFQMRSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNSPTFQMRSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetPrecType for complete further documentation of this routine.

FSUNMASSSPTFQMRSETPRECTYPE

Call FSUNMASSSPTFQMRSETPRECTYPE(pretype, ier)

Description The function FSUNMASSSPTFQMRSETPRECTYPE can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPTFQMRSETPRECTYPE above, except that code is not needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetPrecType for complete further documentation of this routine.

FSUNSPTFQMRSETMAXL

Call FSUNSPTFQMRSETMAXL(code, maxl, ier)

Description The function FSUNSPTFQMRSETMAXL can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments code (int*) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

maxl (int*) the number of iterations to allow.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

FSUNMASSSPTFQMRSETMAXL

Call FSUNMASSSPTFQMRSETMAXL(maxl, ier)

Description The function FSUNMASSSPTFQMRSETMAXL can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPTFQMRSETMAXL above, except that code is not needed since mass matrix linear systems only arise in ARKODE.

Return value ier is a int return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

10.16.4 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;
};
```

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.

10.17 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementaiton of the PCG (Preconditioned Conjugate Gradient [25]) 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.

10.17.1 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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{10.4}$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \tag{10.5}$$

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

$$\begin{aligned} & \|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta \\ \Leftrightarrow \\ & \|SP^{-1}b - SP^{-1}Ax\|_2 < \delta \\ \Leftrightarrow \\ & \|P^{-1}b - P^{-1}Ax\|_S < \delta \end{aligned}$$

where $\|v\|_S = \sqrt{v^T S^T S v}$, with an input tolerance δ.

This solver is constructed to perform the following operations:

- During construction all NVECTOR solver data is allocated, with vectors cloned from a template NVECTOR that is input, and default solver parameters are set.
- User-facing "set" routines may be called to modify default solver parameters.
- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLINSOL_PCG to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s` scaling vector.
- In the "initialize" call, the solver parameters are checked for validity.
- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

10.17.2 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 10.1.1 – 10.1.3:

- `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`

10.17.3 SUNLinearSolver_PCG Fortran interfaces

The SUNLINSOL_PCG module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunlinsol_pcg_mod` FORTRAN module defines interfaces to all SUNLINSOL_PCG C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNLinSol_PCG` is interfaced as `FSUNLinSol_PCG`.

The FORTRAN 2003 SUNLINSOL_PCG interface module can be accessed with the `use` statement, i.e. `use fsunlinsol_pcg_mod`, and linking to the library `libsundials_fsunlinsolpcg_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunlinsol_pcg_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunlinsolpcg_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_PCG module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNPCGINIT

Call `FSUNPCGINIT(code, pretype, maxl, ier)`

Description The function `FSUNPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_PCG module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

FSUNMASSPCGINIT

Call `FSUNMASSPCGINIT(pretype, maxl, ier)`

Description The function `FSUNMASSPCGINIT` can be called for Fortran programs to create a SUNLINSOL_PCG object for mass matrix linear systems.

Arguments
- `pretype` (`int*`) flag indicating desired preconditioning type
- `maxl` (`int*`) flag indicating number of iterations to allow

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* the NVECTOR object has been initialized.

Allowable values for `pretype` and `maxl` are the same as for the C function `SUNLinSol_PCG`.

The `SUNLinSol_PCGSetPrecType` and `SUNLinSol_PCGSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers.

FSUNPCGSETPRECTYPE

Call `FSUNPCGSETPRECTYPE(code, pretype, ier)`

Description The function `FSUNPCGSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning to use.

Arguments
- `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
- `pretype` (`int*`) flag indicating the type of preconditioning to use.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetPrecType` for complete further documentation of this routine.

FSUNMASSPCGSETPRECTYPE

Call `FSUNMASSPCGSETPRECTYPE(pretype, ier)`

Description The function `FSUNMASSPCGSETPRECTYPE` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNPCGSETPRECTYPE` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetPrecType` for complete further documentation of this routine.

`FSUNPCGSETMAXL`

Call `FSUNPCGSETMAXL(code, maxl, ier)`

Description The function `FSUNPCGSETMAXL` can be called for Fortran programs to change the maximum number of iterations to allow.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`maxl` (`int*`) the number of iterations to allow.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetMaxl` for complete further documentation of this routine.

`FSUNMASSPCGSETMAXL`

Call `FSUNMASSPCGSETMAXL(maxl, ier)`

Description The function `FSUNMASSPCGSETMAXL` can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to `FSUNPCGSETMAXL` above, except that `code` is not needed since mass matrix linear systems only arise in ARKODE.

Return value `ier` is a `int` return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

Notes See `SUNLinSol_PCGSetMaxl` for complete further documentation of this routine.

10.17.4 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;
};
```

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.

10.18 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 11

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 11.2.

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 11.1 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 11.1.1 – 11.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 11.1.4. A table of nonlinear solver return codes is given in section 11.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 11.1.6. Section 11.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 11.1.8 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.

11.1 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`.

11.1.1 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 11.2 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 11.2 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`

11.1.2 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 11.1.4 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 11.1.4 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 11.1.4 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 11.1.4 for the definition of `SUNNonlinSolConvTestFn`.
- `ctest_data` (`void*`) is a data pointer passed to `CTestFn` every time it is called.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes SUNNONLINSOL implementations utilizing their own convergence test criteria may set this function to `NULL`.

F2003 Name `FSUNNonlinSolSetConvTestFn`

`SUNNonlinSolSetMaxIters`

Call `retval = SUNNonlinSolSetMaxIters(NLS, maxiters);`

Description The *optional* function `SUNNonlinSolSetMaxIters` sets the maximum number of nonlinear solver iterations. This is typically called by SUNDIALS integrators to define their default iteration limit, but may be adjusted by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
`maxiters` (`int`) the maximum number of nonlinear iterations.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure (e.g., `maxiters` < 1).

F2003 Name `FSUNNonlinSolSetMaxIters`

11.1.3 SUNNonlinearSolver get functions

The following get functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routines to get the current total number of iterations (`SUNNonlinSolGetNumIters`) and number of convergence failures (`SUNNonlinSolGetNumConvFails`) are optional. The routine to get the current nonlinear solver iteration (`SUNNonlinSolGetCurIter`) is required when using the convergence test provided by the SUNDIALS integrator or by the ARKODE and CVODE linear solver interfaces. Otherwise, `SUNNonlinSolGetCurIter` is optional.

`SUNNonlinSolGetNumIters`

Call `retval = SUNNonlinSolGetNumIters(NLS, numiters);`

Description The *optional* function `SUNNonlinSolGetNumIters` returns the total number of nonlinear solver iterations. This is typically called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`numiters` (`long int*`) the total number of nonlinear solver iterations.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolGetNumIters`

`SUNNonlinSolGetCurIter`

Call `retval = SUNNonlinSolGetCurIter(NLS, iter);`

Description The function `SUNNonlinSolGetCurIter` returns the iteration index of the current nonlinear solve. This function is *required* when using SUNDIALS integrator-provided convergence tests or when using a SUNLINSOL spils linear solver; otherwise it is *optional*.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`iter` (`int*`) the nonlinear solver iteration in the current solve starting from zero.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolGetCurIter`

`SUNNonlinSolGetNumConvFails`

Call `retval = SUNNonlinSolGetNumConvFails(NLS, nconvfails);`

Description The *optional* function `SUNNonlinSolGetNumConvFails` returns the total number of nonlinear solver convergence failures. This may be called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object

`nconvfails` (`long int*`) the total number of nonlinear solver convergence failures.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolGetNumConvFails`

11.1.4 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 11.2 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 11.2, SUNDIALS integrators formulate nonlinear systems as a function of the correction to the predicted solution. On each call to the nonlinear system function the integrator will compute and store the current solution based on the input correction. Additionally, the residual will store the value of the ODE right-hand side function or DAE residual used in computing the nonlinear system residual. These stored values are then directly used in the integrator-supplied linear solver setup and solve functions as applicable.

`SUNNonlinSolLSetupFn`

Definition
```
typedef int (*SUNNonlinSolLSetupFn)(booleantype jbad, booleantype* jcur,
                                    void* mem);
```

Purpose These functions are wrappers to the SUNDIALS integrator's function for setting up linear solves with SUNLINSOL modules.

Arguments `jbad` is an input indicating whether the nonlinear solver believes that A has gone stale (`SUNTRUE`) or not (`SUNFALSE`).

`jcur` is an output indicating whether the routine has updated the Jacobian A (`SUNTRUE`) or not (`SUNFALSE`).

`mem` is the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

Notes The `SUNNonlinLSetupFn` function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLINSOL direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLINSOL iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize SUNLINSOL linear solvers, or use SUNLINSOL linear solvers that do not require setup may ignore these functions.

As discussed in the description of `SUNNonlinSolSysFn`, the linear solver setup function assumes that the nonlinear system function has been called prior to the linear solver setup function as the setup will utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

`SUNNonlinSolLSolveFn`

Definition
```
typedef int (*SUNNonlinSolLSolveFn)(N_Vector b, void* mem);
```

Purpose These functions are wrappers to the SUNDIALS integrator's function for solving linear systems with SUNLINSOL modules.

Arguments `b` contains the right-hand side vector for the linear solve on input and the solution to the linear system on output.

`mem` is the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

Notes The `SUNNonlinLSolveFn` function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNONLINSOL implementations that do not require solving this system or do not use SUNLINSOL linear solvers may ignore these functions.

As discussed in the description of `SUNNonlinSolSysFn`, the linear solver solve function assumes that the nonlinear system function has been called prior to the linear solver solve function as the solve may utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

`SUNNonlinSolConvTestFn`

Definition
```
typedef int (*SUNNonlinSolConvTestFn)(SUNNonlinearSolver NLS, N_Vector ycor,
                                      N_Vector del, realtype tol,
                                      N_Vector ewt, void* ctest_data);
```

Purpose These functions are SUNDIALS integrator-specific convergence tests for nonlinear solvers and are typically supplied by each SUNDIALS integrator, but users may supply custom problem-specific versions as desired.

Arguments
`NLS` is the SUNNONLINSOL object.
`ycor` is the current correction (nonlinear iterate).
`del` is the difference between the current and prior nonlinear iterates.
`tol` is the nonlinear solver tolerance.
`ewt` is the weight vector used in computing weighted norms.
`ctest_data` is the data pointer provided to `SUNNonlinSolSetConvTestFn`.

Return value The return value of this routine will be a negative value if an unrecoverable error occurred or one of the following:

SUN_NLS_SUCCESS	the iteration is converged.
SUN_NLS_CONTINUE	the iteration has not converged, keep iterating.
SUN_NLS_CONV_RECVR	the iteration appears to be diverging, try to recover.

Notes The tolerance passed to this routine by SUNDIALS integrators is the tolerance in a weighted root-mean-squared norm with error weight vector `ewt`. SUNNONLINSOL modules utilizing their own convergence criteria may ignore these functions.

11.1.5 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 11.1. Here, negative values correspond to non-recoverable failures, positive values to recoverable failures, and zero to a successful call.

Table 11.1: 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

11.1.6 The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic SUNNONLINSOL module on which all other SUNNONLINSOL implementations are built. The `SUNNonlinearSolver` type is a pointer to a structure containing an implementation-dependent *content* field and an *ops* field. The type `SUNNonlinearSolver` is defined as follows:

```
typedef struct _generic_SUNNonlinearSolver *SUNNonlinearSolver;

struct _generic_SUNNonlinearSolver {
  void *content;
  struct _generic_SUNNonlinearSolver_Ops *ops;
};
```

where the `_generic_SUNNonlinearSolver_Ops` structure is a list of pointers to the various actual nonlinear solver operations provided by a specific implementation. The `_generic_SUNNonlinearSolver_Ops` structure is defined as

```
struct _generic_SUNNonlinearSolver_Ops {
  SUNNonlinearSolver_Type (*gettype)(SUNNonlinearSolver);
  int                     (*initialize)(SUNNonlinearSolver);
  int                     (*setup)(SUNNonlinearSolver, N_Vector, void*);
  int                     (*solve)(SUNNonlinearSolver, N_Vector, N_Vector,
                                   N_Vector, realtype, booleantype, void*);
```

```
  int                    (*free)(SUNNonlinearSolver);
  int                    (*setsysfn)(SUNNonlinearSolver, SUNNonlinSolSysFn);
  int                    (*setlsetupfn)(SUNNonlinearSolver, SUNNonlinSolLSetupFn);
  int                    (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
  int                    (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn,
                                       void*);
  int                    (*setmaxiters)(SUNNonlinearSolver, int);
  int                    (*getnumiters)(SUNNonlinearSolver, long int*);
  int                    (*getcuriter)(SUNNonlinearSolver, int*);
  int                    (*getnumconvfails)(SUNNonlinearSolver, long int*);
};
```

The generic SUNNONLINSOL module defines and implements the nonlinear solver operations defined in Sections 11.1.1 – 11.1.3. 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
```

11.1.7 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 8.1.1 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

11.1.8 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 11.1.1 – 11.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one SUNNONLINSOL module (each with different `SUNNonlinearSolver` internal data representations) in the same code.
3. Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

1. Define and implement additional user-callable "set" routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.
2. Provide additional user-callable "get" routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

To aid in the creation of custom SUNNONLINSOL modules the generic SUNNONLINSOL module provides the utility functions `SUNNonlinSolNewEmpty` and `SUNNonlinsolFreeEmpty`. When used in custom SUNNONLINSOL constructors, the function `SUNNonlinSolNewEmpty` will ease the introduction of any new optional nonlinear solver operations to the SUNNONLINSOL API by ensuring only required operations need to be set.

`SUNNonlinSolNewEmpty`

Call `NLS = SUNNonlinSolNewEmpty();`

Description The function `SUNNonlinSolNewEmpty` allocates a new generic SUNNONLINSOL object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

Arguments None

Return value This function returns a `SUNNonlinearSolver` object. If an error occurs when allocating the object, then this routine will return `NULL`.

F2003 Name `FSUNNonlinSolNewEmpty`

`SUNNonlinSolFreeEmpty`

Call `SUNNonlinSolFreeEmpty(NLS);`

Description This routine frees the generic `SUNNonlinearSolver` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments `NLS` (`SUNNonlinearSolver`)

Return value None

F2003 Name `FSUNNonlinSolFreeEmpty`

11.2 CVODES SUNNonlinearSolver interface

As discussed in Chapter 2 each integration step requires the (approximate) solution of a nonlinear system. This system can be formulated as the rootfinding problem

$$F(y^n) \equiv y^n - h_n \beta_{n,0} f(t_n, y^n) - a_n = 0\,, \tag{11.1}$$

or as the fixed-point problem

$$G(y^n) \equiv h_n \beta_{n,0} f(t_n, y^n) + a_n = y^n\,, \tag{11.2}$$

where $a_n \equiv \sum_{i>0}(\alpha_{n,i} y^{n-i} + h_n \beta_{n,i} \dot{y}^{n-i})$.

Rather than solving the above nonlinear systems for the new state y^n CVODES reformulates the above problems to solve for the correction y_{cor} to the predicted new state y_{pred} so that $y^n = y_{pred} + y_{cor}$. The nonlinear systems rewritten in terms of y_{cor} are

$$F(y_{cor}) \equiv y_{pred} + y_{cor} - h_n \beta_{n,0} f(t_n, y_{pred} + y_{cor}) - a_n = 0\,, \tag{11.3}$$

for the rootfinding problem and

$$G(y_{cor}) \equiv h_n \beta_{n,0} f(t_n, y_{pred} + y_{cor}) + a_n - y_{pred} = y_{cor}\,. \tag{11.4}$$

for the fixed-point problem. Similarly in the forward sensitivity analysis case the combined state and sensitivity nonlinear systems are also reformulated in terms of the correction to the predicted state and sensitivities.

The nonlinear system functions provided by CVODES to the nonlinear solver module internally update the current value of the new state (and the sensitvities) based on the input correction vector. The updated vector(s) are used when calling the ODE right-hand side function and when setting up linear solves (e.g., updating the Jacobian or preconditioner).

CVODES 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 value of γ to compute Jacobian data.

`CVodeGetCurrentGamma`

Call `flag = CVodeGetCurrentGamma(cvode_mem, &gamma);`

Description The function `CVodeGetCurrentGamma` returns the current value of the scalar γ.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODE memory block.
- `gamma` (`realtype *`) the current value of the scalar γ appearing in the Newton equation $M = I - \gamma J$.

Return value The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVodeGetCurrentState`

Call `flag = CVodeGetCurrentState(cvode_mem, &y);`

Description The function `CVodeGetCurrentState` returns the current state vector.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODE memory block.
- `y` (`N_Vector *`) pointer that is set to the current state vector

Return value The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVodeGetCurrentStateSens`

Call `flag = CVodeGetCurrentStateSens(cvode_mem, &yS);`

Description The function `CVodeGetCurrentStateSens` returns the current sensitivity state vector array.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODE memory block.
- `yS` (`N_Vector **`) pointer to the vector array that is set to the current sensitivity state vector array

Return value The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVodeGetCurrentSensSolveIndex`

Call `flag = CVodeGetCurrentSensSolveIndex(cvode_mem, &index);`

Description The function `CVodeGetCurrentSensSolveIndex` returns the index of the current sensitivity solve when using the `CV_STAGGERED1` solver.

Arguments
- `cvode_mem` (`void *`) pointer to the CVODE memory block.
- `index` (`int *`) will be set to the index of the current sensitivity solve

Return value The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

11.3 The SUNNonlinearSolver_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton's method. To access the SUNNONLINSOL_NEWTON module, include the header file `sunnonlinsol/sunnonlinsol_newton.h`. We note that the SUNNONLINSOL_NEWTON module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolnewton` module library.

11.3.1 SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{11.5}$$

given an initial guess $y^{(0)}$, Newton's method computes a series of approximate solutions

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{11.6}$$

where m is the Newton iteration index, and the Newton update $\delta^{(m+1)}$ is the solution of the linear system

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)})\,, \tag{11.7}$$

in which A is the Jacobian matrix

$$A \equiv \partial F/\partial y\,. \tag{11.8}$$

Depending on the linear solver used, the SUNNONLINSOL_NEWTON module will employ either a Modified Newton method, or an Inexact Newton method [7, 10, 18, 20, 37]. When used with a direct linear solver, the Jacobian matrix A is held constant during the Newton iteration, resulting in a Modified Newton method. With a matrix-free iterative linear solver, the iteration is an Inexact Newton method.

In both cases, calls to the integrator-supplied `SUNNonlinSolLSetupFn` function are made infrequently to amortize the increased cost of matrix operations (updating A and its factorization within direct linear solvers, or updating the preconditioner within iterative linear solvers). Specifically, SUNNONLINSOL_NEWTON will call the `SUNNonlinSolLSetupFn` function in two instances:

(a) when requested by the integrator (the input `callLSetSetup` is `SUNTRUE`) before attempting the Newton iteration, or

(b) when reattempting the nonlinear solve after a recoverable failure occurs in the Newton iteration with stale Jacobian information (`jcur` is `SUNFALSE`). In this case, SUNNONLINSOL_NEWTON will set `jbad` to `SUNTRUE` before calling the `SUNNonlinSolLSetupFn` function.

Whether the Jacobian matrix A is fully or partially updated depends on logic unique to each integrator-supplied `SUNNonlinSolSetupFn` routine. We refer to the discussion of nonlinear solver strategies provided in Chapter 2 for details on this decision.

The default maximum number of iterations and the stopping criteria for the Newton iteration are supplied by the SUNDIALS integrator when SUNNONLINSOL_NEWTON is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling the `SUNNonlinSolSetMaxIters` and/or `SUNNonlinSolSetConvTestFn` functions after attaching the SUNNONLINSOL_NEWTON object to the integrator.

11.3.2 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 11.1.1 – 11.1.3 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 11.1.1 – 11.1.3 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`

11.3.3 SUNNonlinearSolver_Newton Fortran interfaces

The SUNNONLINSOL_NEWTON module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunnonlinsol_newton_mod` FORTRAN module defines interfaces to all SUNNONLINSOL_NEWTON C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNNonlinSol_Newton` is interfaced as `FSUNNonlinSol_Newton`.

The FORTRAN 2003 SUNNONLINSOL_NEWTON interface module can be accessed with the `use` statement, i.e. `use fsunnonlinsol_newton_mod`, and linking to the library `libsundials_fsunnonlinsolnewton_mod.`*lib* in addition to the C library. For details on where the

library and module file `fsunnonlinsol_newton_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunnonlinsolnewton_mod` library.

FORTRAN 77 interface functions

For SUNDIALS integrators that include a FORTRAN 77 interface, the SUNNONLINSOL_NEWTON module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

`FSUNNEWTONINIT`

Call `FSUNNEWTONINIT(code, ier);`

Description The function `FSUNNEWTONINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ with Newton's method.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

11.3.4 SUNNonlinearSolver_Newton content

The SUNNONLINSOL_NEWTON module defines the *content* field of a `SUNNonlinearSolver` as the following structure:

```
struct _SUNNonlinearSolverContent_Newton {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolLSetupFn   LSetup;
  SUNNonlinSolLSolveFn   LSolve;
  SUNNonlinSolConvTestFn CTest;

  N_Vector    delta;
  booleantype jcur;
  int         curiter;
  int         maxiters;
  long int    niters;
  long int    nconvfails;
  void*       ctest_data;
};
```

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.

11.4 The SUNNonlinearSolver_FixedPoint implementation

This section describes the SUNNONLINSOL implementation of a fixed point (functional) iteration with optional Anderson acceleration. To access the SUNNONLINSOL_FIXEDPOINT module, include the header file `sunnonlinsol/sunnonlinsol_fixedpoint.h`. We note that the SUNNONLINSOL_FIXEDPOINT module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolfixedpoint` module library.

11.4.1 SUNNonlinearSolver_FixedPoint description

To find the solution to

$$G(y) = y \tag{11.9}$$

given an initial guess $y^{(0)}$, the fixed point iteration computes a series of approximate solutions

$$y^{(n+1)} = G(y^{(n)}) \tag{11.10}$$

where n is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [5, 52, 21, 42]. With Anderson acceleration using subspace size m, the series of approximate solutions can be formulated as the linear combination

$$y^{(n+1)} = \beta \sum_{i=0}^{m_n} \alpha_i^{(n)} G(y^{(n-m_n+i)}) + (1-\beta) \sum_{i=0}^{m_n} \alpha_i^{(n)} y_{n-m_n+i} \tag{11.11}$$

where $m_n = \min\{m, n\}$, β is a damping parameter ($\beta = 1.0$ i.e., no damping by default) and the factors

$$\alpha^{(n)} = (\alpha_0^{(n)}, \ldots, \alpha_{m_n}^{(n)}) \tag{11.12}$$

solve the minimization problem $\min_\alpha \|F_n \alpha^T\|_2$ under the constraint that $\sum_{i=0}^{m_n} \alpha_i = 1$ where

$$F_n = (f_{n-m_n}, \ldots, f_n) \tag{11.13}$$

with $f_i = G(y^{(i)}) - y^{(i)}$. Due to this constraint, in the limit of $m = 0$ the accelerated fixed point iteration formula (11.11) simplifies to the standard fixed point iteration (11.10).

Following the recommendations made in [52], the SUNNONLINSOL_FIXEDPOINT implementation computes the series of approximate solutions as

$$y^{(n+1)} = G(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} - (1-\beta)(f(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta f_{n-m_n+i}) \tag{11.14}$$

with $\Delta g_i = G(y^{(i+1)}) - G(y^{(i)})$ and where the factors

$$\gamma^{(n)} = (\gamma_0^{(n)}, \ldots, \gamma_{m_n-1}^{(n)}) \tag{11.15}$$

solve the unconstrained minimization problem $\min_\gamma \|f_n - \Delta F_n \gamma^T\|_2$ where

$$\Delta F_n = (\Delta f_{n-m_n}, \ldots, \Delta f_{n-1}), \tag{11.16}$$

with $\Delta f_i = f_{i+1} - f_i$. The least-squares problem is solved by applying a QR factorization to $\Delta F_n = Q_n R_n$ and solving $R_n \gamma = Q_n^T f_n$.

The acceleration subspace size m is required when constructing the SUNNONLINSOL_FIXEDPOINT object. The default maximum number of iterations and the stopping criteria for the fixed point iteration are supplied by the SUNDIALS integrator when SUNNONLINSOL_FIXEDPOINT is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling `SUNNonlinSolSetMaxIters` and `SUNNonlinSolSetConvTestFn` functions after attaching the SUNNONLINSOL_FIXEDPOINT object to the integrator.

11.4.2 SUNNonlinearSolver_FixedPoint functions

The SUNNONLINSOL_FIXEDPOINT module provides the following constructors for creating a `SUNNonlinearSolver` object.

`SUNNonlinSol_FixedPoint`

Call `NLS = SUNNonlinSol_FixedPoint(y, m);`

Description The function `SUNNonlinSol_FixedPoint` creates a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.

Arguments `y` (`N_Vector`) a template for cloning vectors needed within the solver
`m` (`int`) the number of acceleration vectors to use

Return value The return value `NLS` (of type `SUNNonlinearSolver`) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise `NLS` will be `NULL`.

F2003 Name `FSUNNonlinSol_FixedPoint`

`SUNNonlinSol_FixedPointSens`

Call `NLS = SUNNonlinSol_FixedPointSens(count, y, m);`

Description The function `SUNNonlinSol_FixedPointSens` creates a `SUNNonlinearSolver` object for use with SUNDIALS sensitivity enabled integrators (CVODES and IDAS) to solve nonlinear systems of the form $G(y) = y$.

Arguments `count` (`int`) the number of vectors in the nonlinear solve. When integrating a system containing `Ns` sensitivities the value of `count` is:

- `Ns+1` if using a *simultaneous* corrector approach.
- `Ns` if using a *staggered* corrector approach.

`y` (`N_Vector`) a template for cloning vectors needed within the solver.
`m` (`int`) the number of acceleration vectors to use.

Return value The return value `NLS` (of type `SUNNonlinearSolver`) will be a SUNNONLINSOL object if the constructor exits successfully, otherwise `NLS` will be `NULL`.

F2003 Name `FSUNNonlinSol_FixedPointSens`

Since the accelerated fixed point iteration (11.10) does not require the setup or solution of any linear systems, the SUNNONLINSOL_FIXEDPOINT module implements all of the functions defined in sections 11.1.1 – 11.1.3 except for the `SUNNonlinSolSetup`, `SUNNonlinSolSetLSetupFn`, and `SUNNonlinSolSetLSolveFn` functions, that are set to `NULL`. The SUNNONLINSOL_FIXEDPOINT functions have the same names as those defined by the generic SUNNONLINSOL API with `_FixedPoint` appended to the function name. Unless using the SUNNONLINSOL_FIXEDPOINT module as a standalone nonlinear solver the generic functions defined in sections 11.1.1 – 11.1.3 should be called in favor of the SUNNONLINSOL_FIXEDPOINT-specific implementations.

The SUNNONLINSOL_FIXEDPOINT module also defines the following additional user-callable functions.

`SUNNonlinSolGetSysFn_FixedPoint`

Call `retval = SUNNonlinSolGetSysFn_FixedPoint(NLS, SysFn);`

Description The function `SUNNonlinSolGetSysFn_FixedPoint` returns the fixed-point function that defines the nonlinear system.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object.
`SysFn` (`SUNNonlinSolSysFn*`) the function defining the nonlinear system.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

Notes This function is intended for users that wish to evaluate the fixed-point function in a custom convergence test function for the SUNNONLINSOL_FIXEDPOINT module. We note that SUNNONLINSOL_FIXEDPOINT will not leverage the results from any user calls to `SysFn`.

F2003 Name `FSUNNonlinSolGetSysFn_FixedPoint`

`SUNNonlinSolSetDamping_FixedPoint`

Call `retval = SUNNonlinSolSetDamping_FixedPoint(NLS, beta);`

Description The function `SUNNonlinSolSetDamping_FixedPoint` sets the damping parameter β to use with Anderson acceleration. By default damping is disabled i.e., $\beta = 1.0$.

Arguments `NLS` (`SUNNonlinearSolver`) a SUNNONLINSOL object
`beta` (`realtype`) the damping parameter $0 < beta \leq 1$.

Return value The return value `retval` (of type `int`) is zero for a successful call, `SUN_NLS_MEM_NULL` if `NLS` is `NULL`, or `SUN_NLS_ILL_INPUT` if `beta` is negative.

Notes A `beta` value should be greater than zero and less than one if damping is to be used. A value of one or more will disable damping.

11.4.3 SUNNonlinearSolver_FixedPoint Fortran interfaces

The SUNNONLINSOL_FIXEDPOINT module provides a FORTRAN 2003 module as well as FORTRAN 77 style interface functions for use from FORTRAN applications.

FORTRAN 2003 interface module

The `fsunnonlinsol_fixedpoint_mod` FORTRAN module defines interfaces to all SUNNONLINSOL_FIXEDPOINT C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading 'F'. For example, the function `SUNNonlinSol_FixedPoint` is interfaced as `FSUNNonlinSol_FixedPoint`.

The FORTRAN 2003 SUNNONLINSOL_FIXEDPOINT interface module can be accessed with the `use` statement, i.e. `use fsunnonlinsol_fixedpoint_mod`, and linking to the library `libsundials_fsunnonlinsolfixedpoint_mod.`*lib* in addition to the C library. For details on where the library and module file `fsunnonlinsol_fixedpoint_mod.mod` are installed see Appendix A. We note that the module is accessible from the FORTRAN 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fsunnonlinsolfixedpoint_mod` library.

FORTRAN 77 interface functions

For SUNDIALS integrators that include a FORTRAN 77 interface, the SUNNONLINSOL_FIXEDPOINT module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

`FSUNFIXEDPOINTINIT`

Call `FSUNFIXEDPOINTINIT(code, m, ier);`

Description The function `FSUNFIXEDPOINTINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE).
`m` (`int*`) is an integer input specifying the number of acceleration vectors.

Return value `ier` is a return completion flag equal to `0` for a success return and `-1` otherwise. See printed message for details in case of failure.

11.4.4 SUNNonlinearSolver_FixedPoint content

The SUNNONLINSOL_FIXEDPOINT module defines the *content* field of a `SUNNonlinearSolver` as the following structure:

```
struct _SUNNonlinearSolverContent_FixedPoint {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolConvTestFn CTest;

  int       m;
  int      *imap;
  realtype *R;
  realtype *gamma;
  realtype *cvals;
  N_Vector *df;
  N_Vector *dg;
  N_Vector *q;
  N_Vector *Xvecs;
  N_Vector  yprev;
  N_Vector  gy;
  N_Vector  fold;
  N_Vector  gold;
  N_Vector  delta;
  int       curiter;
  int       maxiters;
  long int  niters;
  long int  nconvfails;
  void*     ctest_data;
};
```

The following entries of the *content* field are always allocated:

`Sys` - function for evaluating the nonlinear system,

`CTest` - function for checking convergence of the fixed point iteration,

`yprev` - `N_Vector` used to store previous fixed-point iterate,

`gy` - `N_Vector` used to store $G(y)$ in fixed-point algorithm,

`delta` - `N_Vector` used to store difference between successive fixed-point iterates,

`curiter` - the current number of iterations in the solve attempt,

`maxiters` - the maximum number of fixed-point iterations allowed in a solve,

`niters` - the total number of nonlinear iterations across all solves,

`nconvfails` - the total number of nonlinear convergence failures across all solves,

`ctest_data` - the data pointer passed to the convergence test function, and

`m` - number of acceleration vectors,

If Anderson acceleration is requested (i.e., $m > 0$ in the call to `SUNNonlinSol_FixedPoint`), then the following items are also allocated within the *content* field:

`imap` - index array used in acceleration algorithm (length `m`),

`damping` - a flag indicating if damping is enabled,

`beta` - the damping parameter,

`R` - small matrix used in acceleration algorithm (length `m*m`),

`gamma` - small vector used in acceleration algorithm (length `m`),

`cvals` - small vector used in acceleration algorithm (length `m+1`),

`df` - array of `N_Vectors` used in acceleration algorithm (length `m`),

`dg` - array of `N_Vectors` used in acceleration algorithm (length `m`),

`q` - array of `N_Vectors` used in acceleration algorithm (length `m`),

`Xvecs` - `N_Vector` pointer array used in acceleration algorithm (length `m+1`),

`fold` - `N_Vector` used in acceleration algorithm, and

`gold` - `N_Vector` used in acceleration algorithm.

11.5 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 8.8 which discusses the NVECTOR interface to the PETSc Vec API.

11.5.1 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 [6].

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.

11.5.2 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 11.1.1 – 11.1.3 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 11.1.1 – 11.1.3 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.

11.5.3 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.

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.

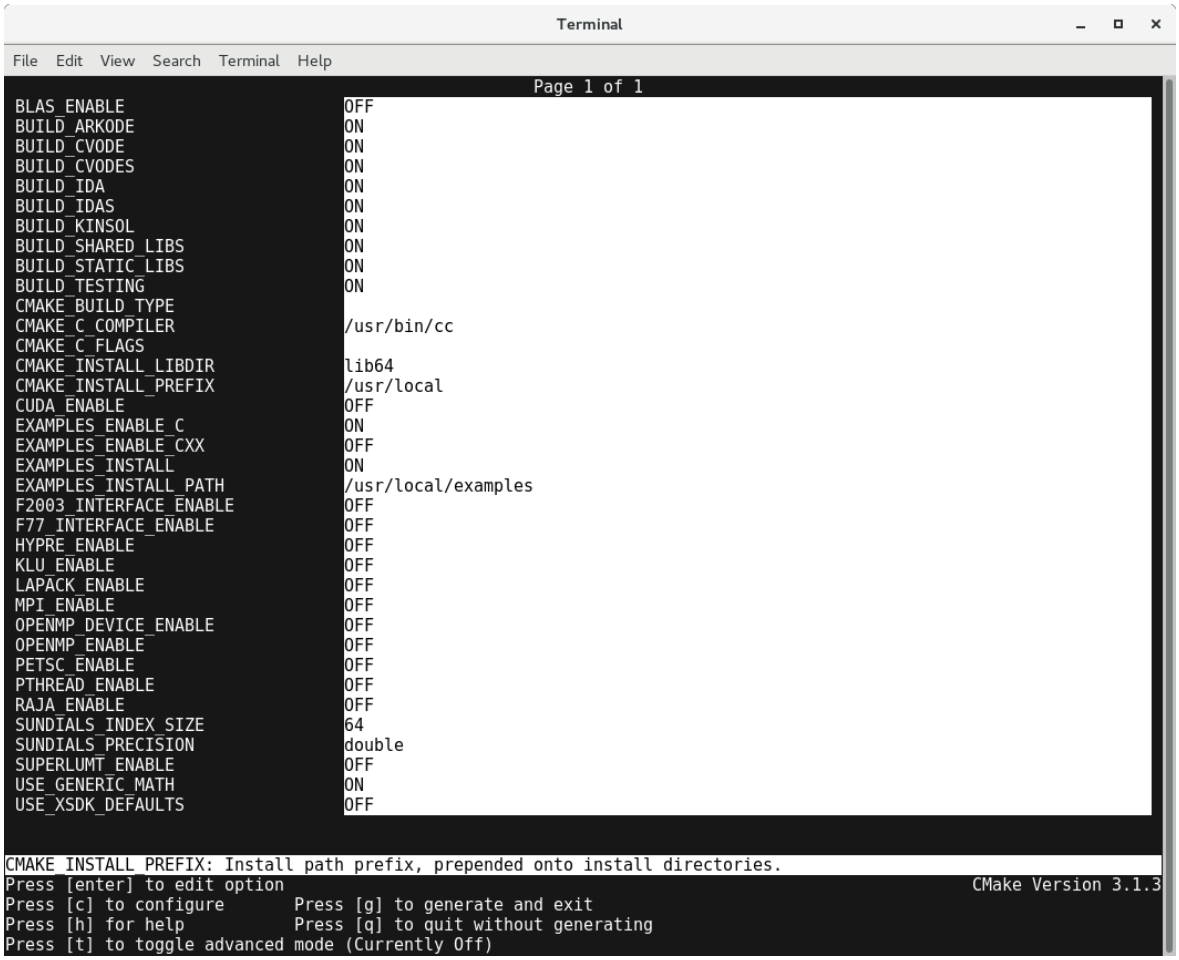

Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

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:

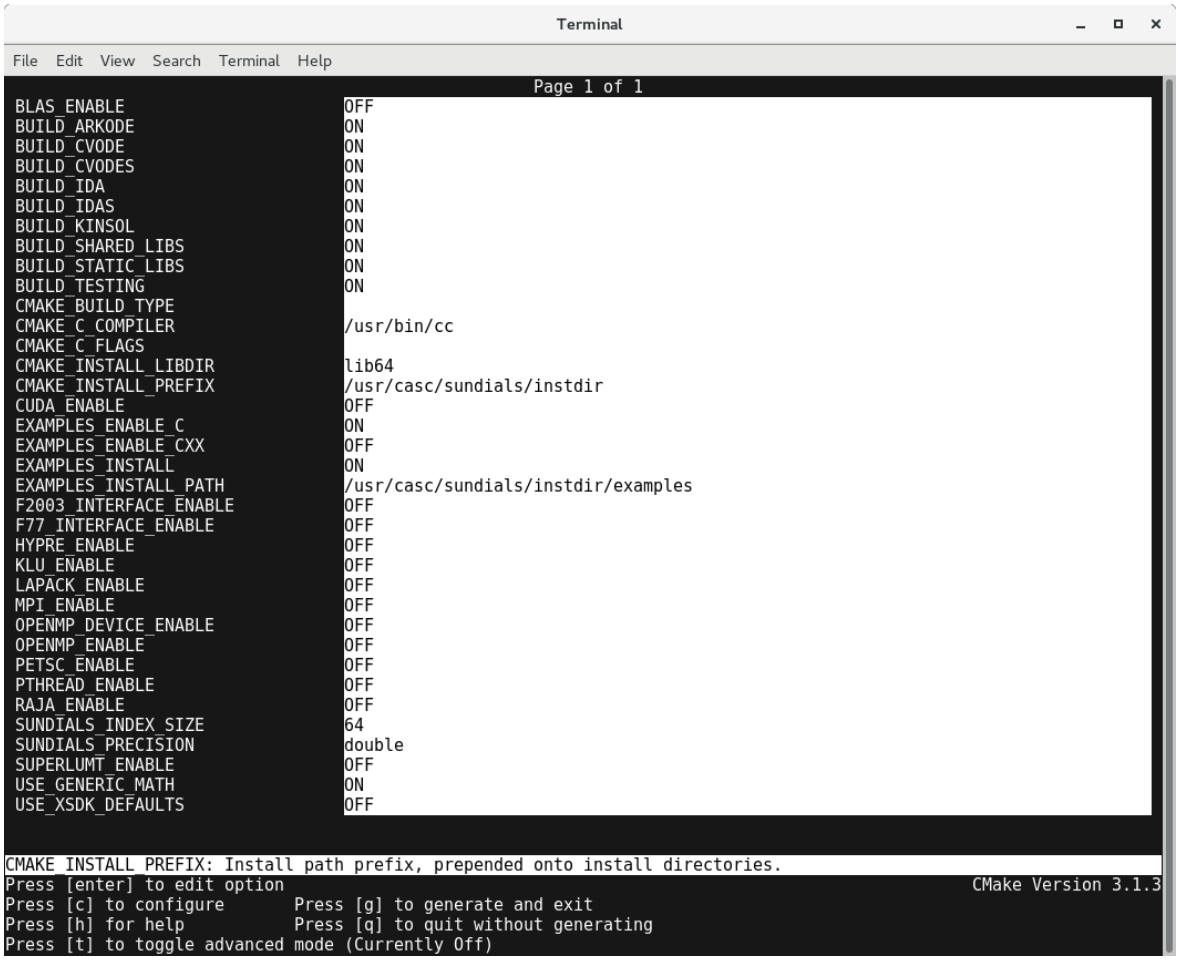

Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

```
% make
```

To install SUNDIALS in the installation directory specified in the configuration, simply run:

```
% make install
```

Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the `cmake` command. The following will build the default configuration:

```
% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../solverdir
% make
% make install
```

A.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

`BUILD_ARKODE` - Build the ARKODE library
Default: ON

`BUILD_CVODE` - Build the CVODE library
Default: ON

`BUILD_CVODES` - Build the CVODES library
Default: ON

`BUILD_IDA` - Build the IDA library
Default: ON

`BUILD_IDAS` - Build the IDAS library
Default: ON

`BUILD_KINSOL` - Build the KINSOL library
Default: ON

`BUILD_SHARED_LIBS` - Build shared libraries
Default: ON

`BUILD_STATIC_LIBS` - Build static libraries
Default: ON

`CMAKE_BUILD_TYPE` - Choose the type of build, options are: `None` (CMAKE_C_FLAGS used), `Debug`, `Release`, `RelWithDebInfo`, and `MinSizeRel`
Default:
Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by CMAKE_<language>_FLAGS.

`CMAKE_C_COMPILER` - C compiler
Default: /usr/bin/cc

`CMAKE_C_FLAGS` - Flags for C compiler
Default:

`CMAKE_C_FLAGS_DEBUG` - Flags used by the C compiler during debug builds
Default: -g

`CMAKE_C_FLAGS_MINSIZEREL` - Flags used by the C compiler during release minsize builds
Default: -Os -DNDEBUG

`CMAKE_C_FLAGS_RELEASE` - Flags used by the C compiler during release builds
Default: -O3 -DNDEBUG

`CMAKE_CXX_COMPILER` - C++ compiler
Default: /usr/bin/c++
Note: A C++ compiler (and all related options) are only triggered if C++ examples are enabled (`EXAMPLES_ENABLE_CXX` is ON). All SUNDIALS solvers can be used from C++ applications by default without setting any additional configuration options.

`CMAKE_CXX_FLAGS` - Flags for C++ compiler
Default:

`CMAKE_CXX_FLAGS_DEBUG` - Flags used by the C++ compiler during debug builds
Default: -g

`CMAKE_CXX_FLAGS_MINSIZEREL` - Flags used by the C++ compiler during release minsize builds
Default: -Os -DNDEBUG

CMAKE_CXX_FLAGS_RELEASE - Flags used by the C++ compiler during release builds
Default: -O3 -DNDEBUG

CMAKE_Fortran_COMPILER - Fortran compiler
Default: /usr/bin/gfortran
Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (FCMIX_ENABLE is ON) or LAPACK support is enabled (LAPACK_ENABLE is ON).

CMAKE_Fortran_FLAGS - Flags for Fortran compiler
Default:

CMAKE_Fortran_FLAGS_DEBUG - Flags used by the Fortran compiler during debug builds
Default: -g

CMAKE_Fortran_FLAGS_MINSIZEREL - Flags used by the Fortran compiler during release minsize builds
Default: -Os

CMAKE_Fortran_FLAGS_RELEASE - Flags used by the Fortran compiler during release builds
Default: -O3

CMAKE_INSTALL_PREFIX - Install path prefix, prepended onto install directories
Default: /usr/local
Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories include and CMAKE_INSTALL_LIBDIR of CMAKE_INSTALL_PREFIX, respectively.

CMAKE_INSTALL_LIBDIR - Library installation directory
Default:
Note: This is the directory within CMAKE_INSTALL_PREFIX that the SUNDIALS libraries will be installed under. The default is automatically set based on the operating system using the GNUInstallDirs CMake module.

Fortran_INSTALL_MODDIR - Fortran module installation directory
Default: fortran

CUDA_ENABLE - Build the SUNDIALS CUDA 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 Trilinos_ENABLE is ON.

EXAMPLES_ENABLE_F77 - Build the SUNDIALS Fortran77 examples
Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F90 - Build the SUNDIALS Fortran90 examples
Default: ON (if F77_INTERFACE_ENABLE is ON)

EXAMPLES_ENABLE_F2003 - Build the SUNDIALS Fortran2003 examples
Default: ON (if F2003_INTERFACE_ENABLE is ON)

EXAMPLES_INSTALL - Install example files
Default: ON
Note: This option is triggered when any of the SUNDIALS example programs are enabled (EXAMPLES_ENABLE_<language> is ON). If the user requires installation of example programs then the sources and sample output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by EXAMPLES_INSTALL_PATH. A CMake configuration script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by EXAMPLES_INSTALL_PATH.

EXAMPLES_INSTALL_PATH - Output directory for installing example files
Default: /usr/local/examples
Note: The actual default value for this option will be an examples subdirectory created under CMAKE_INSTALL_PREFIX.

F77_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 77 interfaces
Default: OFF

F2003_INTERFACE_ENABLE - Enable Fortran-C support via the Fortran 2003 interfaces
Default: OFF

HYPRE_ENABLE - Enable *hypre* support
Default: OFF
Note: See additional information on building with *hypre* enabled in A.1.4.

HYPRE_INCLUDE_DIR - Path to *hypre* header files

HYPRE_LIBRARY_DIR - Path to *hypre* installed library files

KLU_ENABLE - Enable KLU support
Default: OFF
Note: See additional information on building with KLU enabled in A.1.4.

KLU_INCLUDE_DIR - Path to SuiteSparse header files

KLU_LIBRARY_DIR - Path to SuiteSparse installed library files

LAPACK_ENABLE - Enable LAPACK support
Default: OFF
Note: Setting this option to ON will trigger additional CMake options. See additional information on building with LAPACK enabled in A.1.4.

LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

MPI_ENABLE - Enable MPI support. This will build the parallel NVECTOR and the MPI-aware version of the ManyVector library.
Default: OFF
Note: Setting this option to ON will trigger several additional options related to MPI.

MPI_C_COMPILER - mpicc program
Default:

MPI_CXX_COMPILER - mpicxx program
Default:

Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON) and C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than MPI_ENABLE.

MPI_Fortran_COMPILER - mpif77 or mpif90 program
Default:
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON) and Fortran-C support is enabled (F77_INTERFACE_ENABLE or F2003_INTERFACE_ENABLE is ON).

MPIEXEC_EXECUTABLE - Specify the executable for running MPI programs
Default: mpirun
Note: This option is triggered only if MPI is enabled (MPI_ENABLE is ON).

OPENMP_ENABLE - Enable OpenMP support (build the OpenMP NVECTOR).
Default: OFF

OPENMP_DEVICE_ENABLE - Enable OpenMP device offloading (build the OpenMPDEV nvector) if supported by the provided compiler.
Default: OFF

SKIP_OPENMP_DEVICE_CHECK - **advanced option** - Skip the check done to see if the OpenMP provided by the compiler supports OpenMP device offloading.
Default: OFF

PETSC_ENABLE - Enable PETSc support
Default: OFF
Note: See additional information on building with PETSc enabled in **??**.

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:

PTHREAD_ENABLE - Enable Pthreads support (build the Pthreads NVECTOR).
Default: OFF

RAJA_ENABLE - Enable RAJA support (build the RAJA NVECTOR).
Default: OFF
Note: You need to enable CUDA in order to build the RAJA vector module.

SUNDIALS_F77_FUNC_CASE - **advanced option** - Specify the case to use in the Fortran name-mangling scheme, options are: lower or upper
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (lower) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_UNDERSCORES must also be set.

SUNDIALS_F77_FUNC_UNDERSCORES - **advanced option** - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: none, one, or two
Default:
Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available

or to override the inferred or default (one) scheme if one can not be determined. If used, SUNDIALS_F77_FUNC_CASE must also be set.

SUNDIALS_INDEX_TYPE - **advanced option** - Integer type used for SUNDIALS indices. The size must match the size provided for the
SUNDIALS_INDEX_SIZE option.
Default:
Note: In past SUNDIALS versions, a user could set this option to INT64_T to use 64-bit integers, or INT32_T to use 32-bit integers. Starting in SUNDIALS 3.2.0, these special values are deprecated. For SUNDIALS 3.2.0 and up, a user will only need to use the SUNDIALS_INDEX_SIZE option in most cases.

SUNDIALS_INDEX_SIZE - Integer size (in bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 64
Note: The build system tries to find an integer type of appropriate size. Candidate 64-bit integer types are (in order of preference): int64_t, __int64, long long, and long. Candidate 32-bit integers are (in order of preference): int32_t, int, and long. The advanced option, SUNDIALS_INDEX_TYPE can be used to provide a type not listed here.

SUNDIALS_PRECISION - Precision used in SUNDIALS, options are: double, single, or extended
Default: double

SUPERLUDIST_ENABLE - Enable SuperLU_DIST support
Default: OFF
Note: See additional information on building with SuperLU_DIST enabled in A.1.4.

SUPERLUDIST_INCLUDE_DIR - Path to SuperLU_DIST header files (typically SRC directory)

SUPERLUDIST_LIBRARY_DIR - Path to SuperLU_DIST installed library files

SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST

SUPERLUDIST_OpenMP - Enable SUNDIALS support for SuperLU_DIST built with OpenMP
Default: OFF
Note: SuperLU_DIST must be built with OpenMP support for this option to function properly. Additionally the environment variable OMP_NUM_THREADS must be set to the desired number of threads.

SUPERLUMT_ENABLE - Enable SUPERLUMT support
Default: OFF
Note: See additional information on building with SUPERLUMT enabled in A.1.4.

SUPERLUMT_INCLUDE_DIR - Path to SuperLU_MT header files (typically SRC directory)

SUPERLUMT_LIBRARY_DIR - Path to SuperLU_MT installed library files

SUPERLUMT_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_MT

SUPERLUMT_THREAD_TYPE - Must be set to Pthread or OpenMP
Default: Pthread

Trilinos_ENABLE - Enable Trilinos support (build the Tpetra NVECTOR).
Default: OFF

Trilinos_DIR - Path to the Trilinos install directory.
Default:

TRILINOS_INTERFACE_C_COMPILER - **advanced option** - Set the C compiler for building the Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).
Default: The C compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_COMPILER or MPI_C_COMPILER if USE_XSDK_DEFAULTS=ON.
Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_C_COMPILER_FLAGS - **advanced option** - Set the C compiler flags for Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).
Default: The C compiler flags exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_C_FLAGS if USE_XSDK_DEFAULTS=ON.
Note: It is recommended to use the same flags that were used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER - **advanced option** - Set the C++ compiler for builing Trilinos interface (i.e., NVECTOR_TRILINOS and the examples that use it).
Default: The C++ compiler exported from the found Trilinos installation if USE_XSDK_DEFAULTS=OFF. CMAKE_CXX_COMPILER or MPI_CXX_COMPILER if USE_XSDK_DEFAULTS=ON.
Note: It is recommended to use the same compiler that was used to build the Trilinos library.

TRILINOS_INTERFACE_CXX_COMPILER_FLAGS - **advanced option** - Set the C++ compiler flags for 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.

USE_GENERIC_MATH - Use generic (stdc) math libraries
Default: ON

xSDK Configuration Options

SUNDIALS supports CMake configuration options defined by the Extreme-scale Scientific Software Development Kit (xSDK) community policies (see https://xsdk.info for more information). xSDK CMake options are unused by default but may be activated by setting USE_XSDK_DEFAULTS to ON.

When xSDK options are active, they will overwrite the corresponding SUNDIALS option and may have different default values (see details below). As such the equivalent SUNDIALS options should not be used when configuring with xSDK options. In the GUI front end to CMake (ccmake), setting USE_XSDK_DEFAULTS to ON will hide the corresponding SUNDIALS options as advanced CMake variables. During configuration, messages are output detailing which xSDK flags are active and the equivalent SUNDIALS options that are replaced. Below is a complete list xSDK options and the corresponding SUNDIALS options if applicable.

TPL_ENABLE_HYPRE - Enable *hypre* support
Default: OFF
SUNDIALS equivalent: HYPRE_ENABLE

TPL_ENABLE_KLU - Enable KLU support
Default: OFF
SUNDIALS equivalent: KLU_ENABLE

TPL_ENABLE_PETSC - Enable PETSc support
Default: OFF
SUNDIALS equivalent: PETSC_ENABLE

TPL_ENABLE_LAPACK - Enable LAPACK support
Default: OFF
SUNDIALS equivalent: LAPACK_ENABLE

TPL_ENABLE_SUPERLUDIST - Enable SuperLU_DIST support
Default: OFF
SUNDIALS equivalent: SUPERLUDIST_ENABLE

TPL_ENABLE_SUPERLUMT - Enable SuperLU_MT support
Default: OFF
SUNDIALS equivalent: SUPERLUMT_ENABLE

TPL_HYPRE_INCLUDE_DIRS - Path to *hypre* header files
SUNDIALS equivalent: HYPRE_INCLUDE_DIR

TPL_HYPRE_LIBRARIES - *hypre* library
SUNDIALS equivalent: N/A

TPL_KLU_INCLUDE_DIRS - Path to KLU header files
SUNDIALS equivalent: KLU_INCLUDE_DIR

TPL_KLU_LIBRARIES - KLU library
SUNDIALS equivalent: N/A

TPL_LAPACK_LIBRARIES - LAPACK (and BLAS) libraries
Default: /usr/lib/liblapack.so;/usr/lib/libblas.so
SUNDIALS equivalent: LAPACK_LIBRARIES
Note: CMake will search for libraries in your LD_LIBRARY_PATH prior to searching default system paths.

TPL_PETSC_DIR - Path to PETSc installation
SUNDIALS equivalent: PETSC_DIR

TPL_SUPERLUDIST_INCLUDE_DIRS - Path to SuperLU_DIST header files
SUNDIALS equivalent: SUPERLUDIST_INCLUDE_DIR

TPL_SUPERLUDIST_LIBRARIES - Semi-colon separated list of libraries needed for SuperLU_DIST including the SuperLU_DIST library itself
SUNDIALS equivalent: SUPERLUDIST_LIBRARIES

TPL_SUPERLUDIST_OPENMP - Enable SUNDIALS support for SuperLU_DIST built with OpenMP
SUNDIALS equivalent: SUPERLUDIST_OPENMP

TPL_SUPERLUMT_LIBRARIES - SuperLU_MT library
SUNDIALS equivalent: N/A

TPL_SUPERLUMT_THREAD_TYPE - SuperLU_MT library thread type
SUNDIALS equivalent: SUPERLUMT_THREAD_TYPE

USE_XSDK_DEFAULTS - Enable xSDK default configuration settings
Default: OFF
SUNDIALS equivalent: N/A
Note: Enabling xSDK defaults also sets CMAKE_BUILD_TYPE to Debug

XSDK_ENABLE_FORTRAN - Enable SUNDIALS Fortran interfaces
Default: OFF
SUNDIALS equivalent: F77_INTERFACE_ENABLE/F2003_INTERFACE_ENABLE

XSDK_INDEX_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64
Default: 32
SUNDIALS equivalent: SUNDIALS_INDEX_SIZE

XSDK_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad
Default: double
SUNDIALS equivalent: SUNDIALS_PRECISION

A.1.3 Configuration examples

The following examples will help demonstrate usage of the CMake configure options.
To configure SUNDIALS using the default C and Fortran compilers, and default `mpicc` and `mpif77` parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of `/home/myname/sundials/`, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> /home/myname/sundials/solverdir
%
% make install
%
```

To disable installation of the examples, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/solverdir
%
% make install
%
```

A.1.4 Working with external Libraries

The SUNDIALS suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries. When building SUNDIALS as a shared library 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 `LAPACK_ENABLE` option to `ON`. If the directory containing the LAPACK library is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `LAPACK_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the `LAPACK_LIBRARIES` variable can be set to the desired libraries rquired for LAPACK.

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DLAPACK_ENABLE=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 5.3.0. To enable KLU, set KLU_ENABLE to ON, set KLU_INCLUDE_DIR to the include path of the KLU installation and set KLU_LIBRARY_DIR to the lib path of the KLU installation. The CMake configure will result in populating the following variables: AMD_LIBRARY, AMD_LIBRARY_DIR, BTF_LIBRARY, BTF_LIBRARY_DIR, COLAMD_LIBRARY, COLAMD_LIBRARY_DIR, and KLU_LIBRARY.

Building with SuperLU_MT

The SuperLU_MT libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/∼xiaoye/SuperLU/#superlu_mt. SUNDIALS has been tested with SuperLU_MT version 3.1. To enable SuperLU_MT, set SUPERLUMT_ENABLE to ON, set SUPERLUMT_INCLUDE_DIR to the SRC path of the SuperLU_MT installation, and set the variable SUPERLUMT_LIBRARY_DIR to the lib path of the SuperLU_MT installation. At the same time, the variable SUPERLUMT_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 OPENMP_ENABLE or PTHREAD_ENABLE set to ON then SuperLU_MT should be set to use the same threading type.

Building with SuperLU_DIST

The SuperLU_DIST libraries are available for download from the Lawrence Berkeley National Laboratory website: http://crd-legacy.lbl.gov/∼xiaoye/SuperLU/#superlu_dist. SUNDIALS has been tested with SuperLU_DIST 6.1.1. To enable SuperLU_DIST, set SUPERLUDIST_ENABLE to ON, set SUPERLUDIST_INCLUDE_DIR to the include directory of the SuperLU_DIST installation (typically SRC), and set the variable

SUPERLUDIST_LIBRARY_DIR to the path to library directory of the SuperLU_DIST installation (typically lib). At the same time, the variable SUPERLUDIST_LIBRARIES must be set to a semi-colon separated list of other libraries SuperLU_DIST depends on. For example, if SuperLU_DIST was built with LAPACK, then include the LAPACK library in this list. If SuperLU_DIST was built with OpenMP support, then you may set SUPERLUDIST_OPENMP to ON to utilize the OpenMP functionality of SuperLU_DIST.

Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having PTHREAD_ENABLE set to ON then SuperLU_DIST should not be set to use OpenMP.

Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: http://www.mcs.anl.gov/
SUNDIALS has been tested with PETSc version 3.10.0–3.12.1. To enable PETSc, set PETSC_ENABLE 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 2.14.0–2.18.0. To enable *hypre*, set `HYPRE_ENABLE` to `ON`, set `HYPRE_INCLUDE_DIR` to the `include` path of the *hypre* installation, and set the variable `HYPRE_LIBRARY_DIR` to the `lib` path of the *hypre* installation.

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 10.1 of the CUDA toolkit. To build them, you need to install the Toolkit and compatible NVIDIA drivers. Both are available for download from the NVIDIA website: `https://developer.nvidia.com/cuda-downloads`. To enable CUDA, set `CUDA_ENABLE` to `ON`. If CUDA is installed in a nonstandard location, you may be prompted to set the variable `CUDA_TOOLKIT_ROOT_DIR` with your CUDA Toolkit installation path. To enable CUDA examples, set `EXAMPLES_ENABLE_CUDA` to `ON`.

Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from `https://github.com/LLNL/RAJA`. SUNDIALS RAJA modules and examples have been tested with RAJA up to version 0.9. Building SUNDIALS RAJA modules requires a CUDA-enabled RAJA installation. To enable RAJA, set `CUDA_ENABLE` and `RAJA_ENABLE` to `ON`. If RAJA is installed in a nonstandard location you will be prompted to set the variable `RAJA_DIR` with the path to the RAJA CMake configuration file. To enable building the RAJA examples set `EXAMPLES_ENABLE_CUDA` to `ON`.

Building with Trilinos

Trilinos is a suite of numerical libraries developed by Sandia National Laboratories. It can be obtained at `https://github.com/trilinos/Trilinos`. SUNDIALS Trilinos modules and examples have been tested with Trilinos version 12.14.1. To enable Trilinos, set `Trilinos_ENABLE` to `ON`. If Trilinos is installed in a nonstandard location you will be prompted to set the variable `Trilinos_DIR` with the path to the Trilinos CMake configuration file. It is desireable to build the Trilinos vector interface with same compiler and options that were used to build Trilinos. CMake will try to find the correct compiler settings automatically from the Trilinos configuration file. If that is not successful, the compilers and options can be manually set with the following CMake variables:

- `Trilinos_INTERFACE_C_COMPILER`
- `Trilinos_INTERFACE_C_COMPILER_FLAGS`
- `Trilinos_INTERFACE_CXX_COMPILER`
- `Trilinos_INTERFACE_CXX_COMPILER_FLAGS`

A.1.5 Testing the build and installation

If SUNDIALS was configured with `EXAMPLES_ENABLE_<language>` options to `ON`, then a set of regression tests can be run after building with the `make` command by running:

```
% make test
```

Additionally, if `EXAMPLES_INSTALL` was also set to `ON`, then a set of smoke tests can be run after installing with the `make install` command by running:

```
% make test_install
```

A.2 Building and Running Examples

Each of the SUNDIALS solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set at least of the `EXAMPLES_ENABLE_<language>` options to `ON`, and set `EXAMPLES_INSTALL` to `ON`. Specify the installation path for the examples with the variable `EXAMPLES_INSTALL_PATH`. CMake will generate `CMakeLists.txt` configuration files (and `Makefile` files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

Either the `CMakeLists.txt` file or the traditional `Makefile` may be used to build the examples as well as serve as a template for creating user developed solutions. To use the supplied `Makefile` simply run `make` to compile and generate the executables. To use CMake from within the installed example directory, run `cmake` (or `ccmake` to use the GUI) followed by `make` to compile the example code. Note that if CMake is used, it will overwrite the traditional `Makefile` with a new CMake-generated `Makefile`. The resulting output from running the examples can be compared with example output bundled in the SUNDIALS distribution.

NOTE: There will potentially be differences in the output due to machine architecture, compiler versions, use of third party libraries etc.

A.3 Configuring, building, and installing on Windows

CMake can also be used to build SUNDIALS on Windows. To build SUNDIALS for use with Visual Studio the following steps should be performed:

1. Unzip the downloaded tar file(s) into a directory. This will be the *solverdir*
2. Create a separate *builddir*
3. Open a Visual Studio Command Prompt and cd to *builddir*
4. Run cmake-gui *../solverdir*
   (a) Hit Configure
   (b) Check/Uncheck solvers to be built
   (c) Change CMAKE_INSTALL_PREFIX to *instdir*
   (d) Set other options as desired
   (e) Hit Generate
5. Back in the VS Command Window:
   (a) Run msbuild ALL_BUILD.vcxproj
   (b) Run msbuild INSTALL.vcxproj

The resulting libraries will be in the *instdir*. The SUNDIALS project can also now be opened in Visual Studio. Double click on the ALL_BUILD.vcxproj file to open the project. Build the whole *solution* to create the SUNDIALS libraries. To use the SUNDIALS libraries in your own projects, you must set the include directories for your project, add the SUNDIALS libraries to your project solution, and set the SUNDIALS libraries as dependencies for your project.

A.4 Installed libraries and exported header files

Using the CMake SUNDIALS build system, the command

```
% make install
```

will install the libraries under *libdir* and the public header files under *includedir*. The values for these directories are *instdir*/CMAKE_INSTALL_LIBDIR and *instdir*/include, respectively. The location can be changed by setting the CMake variable CMAKE_INSTALL_PREFIX. Although all installed libraries reside under *libdir*/CMAKE_INSTALL_LIBDIR, the public header files are further organized into subdirectories under *includedir*/include.

The installed libraries and exported header files are listed for reference in Table A.1. The file extension *.lib* is typically .so for shared libraries and .a for static libraries. Note that, in the Tables, names are relative to *libdir* for libraries and to *includedir* for header files.

A typical user program need not explicitly include any of the shared SUNDIALS header files from under the *includedir*/include/sundials directory since they are explicitly included by the appropriate solver header files (*e.g.*, cvode_dense.h includes sundials_dense.h). However, it is both legal and safe to do so, and would be useful, for example, if the functions declared in sundials_dense.h are to be used in building a preconditioner.

Table A.1: SUNDIALS libraries and header files

SHARED	Libraries	n/a
	Header files	sundials/sundials_config.h sundials/sundials_fconfig.h sundials/sundials_types.h sundials/sundials_math.h sundials/sundials_nvector.h sundials/sundials_fnvector.h sundials/sundials_matrix.h sundials/sundials_linearsolver.h sundials/sundials_iterative.h sundials/sundials_direct.h sundials/sundials_dense.h sundials/sundials_band.h sundials/sundials_nonlinearsolver.h sundials/sundials_version.h sundials/sundials_mpi_types.h
NVECTOR_SERIAL	Libraries	libsundials_nvecserial.*lib* libsundials_fnvecserial_mod.*lib* libsundials_fnvecserial.a
	Header files	nvector/nvector_serial.h
	Module files	fnvector_serial_mod.mod
NVECTOR_PARALLEL	Libraries	libsundials_nvecparallel.*lib* libsundials_fnvecparallel.a 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
NVECTOR_MPIPLUSX	Libraries	libsundials_nvecmpiplusx.*lib* libsundials_nvecmpiplusx_mod.*lib*

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	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/cuda/ThreadPartitioning.hpp nvector/cuda/Vector.hpp nvector/cuda/VectorKernels.cuh
NVECTOR_RAJA	Libraries	libsundials_nveccudaraja.*lib*
	Header files	nvector/nvector_raja.h nvector/raja/Vector.hpp
NVECTOR_TRILINOS	Libraries	libsundials_nvectrilinos.*lib*
	Header files	nvector/nvector_trilinos.h nvector/trilinos/SundialsTpetraVectorInterface.hpp nvector/trilinos/SundialsTpetraVectorKernels.hpp
SUNMATRIX_BAND	Libraries	libsundials_sunmatrixband.*lib* libsundials_fsunmatrixband_mod.*lib* libsundials_fsunmatrixband.a
	Header files	sunmatrix/sunmatrix_band.h
	Module files	fsunmatrix_band_mod.mod
SUNMATRIX_DENSE	Libraries	libsundials_sunmatrixdense.*lib* libsundials_fsunmatrixdense_mod.*lib* libsundials_fsunmatrixdense.a

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	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_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* libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module files	fsunlinsol_pcg_mod.mod
SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs.*lib*
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		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* libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod.*lib*
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h
	Module files	fsunnonlinsol_fixedpoint_mod.mod
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SUNNONLINSOL_PETSCSNES	Libraries	libsundials_sunnonlinsolpetscsnes.*lib*	
	Header files	sunnonlinsol/sunnonlinsol_petscsnes.h	
CVODE	Libraries	libsundials_cvode.*lib* libsundials_fcvode.a libsundials_fcvode_mod.*lib*	
	Header files	cvode/cvode.h cvode/cvode_direct.h cvode/cvode_spils.h cvode/cvode_bbdpre.h	cvode/cvode_impl.h cvode/cvode_ls.h cvode/cvode_bandpre.h
	Module files	fcvode_mod.mod	
CVODES	Libraries	libsundials_cvodes.*lib* libsundials_fcvodes_mod.*lib*	
	Header files	cvodes/cvodes.h cvodes/cvodes_direct.h cvodes/cvodes_spils.h cvodes/cvodes_bbdpre.h	cvodes/cvodes_impl.h cvodes/cvodes_ls.h cvodes/cvodes_bandpre.h
	Module files	fcvodes_mod.mod	
ARKODE	Libraries	libsundials_arkode.*lib* libsundials_farkode.a libsundials_farkode_mod.*lib*	
	Header files	arkode/arkode.h arkode/arkode_ls.h arkode/arkode_bbdpre.h	arkode/arkode_impl.h arkode/arkode_bandpre.h
	Module files	farkode_mod.mod farkode_erkstep_mod.mod	farkode_arkstep_mod.mod farkode_mristep_mod.mod
IDA	Libraries	libsundials_ida.*lib* libsundials_fida.a libsundials_fida_mod.*lib*	
	Header files	ida/ida.h ida/ida_direct.h ida/ida_spils.h	ida/ida_impl.h ida/ida_ls.h ida/ida_bbdpre.h
	Module files	fida_mod.mod	
IDAS	Libraries	libsundials_idas.*lib* libsundials_fidas_mod.*lib*	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_spils.h	idas/idas_impl.h idas/idas_ls.h idas/idas_bbdpre.h
	Module files	fidas_mod.mod	

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KINSOL	Libraries	libsundials_kinsol.*lib* libsundials_fkinsol.a libsundials_fkinsol_mod.*lib*	
	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_spils.h	kinsol/kinsol_impl.h kinsol/kinsol_ls.h kinsol/kinsol_bbdpre.h
	Module files	fkinsol_mod.mod	

Appendix B

CVODES 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 CVODES input constants

CVODES **main solver module**		
CV_ADAMS	1	Adams-Moulton linear multistep method.
CV_BDF	2	BDF linear multistep method.
CV_NORMAL	1	Solver returns at specified output time.
CV_ONE_STEP	2	Solver returns after each successful step.
CV_SIMULTANEOUS	1	Simultaneous corrector forward sensitivity method.
CV_STAGGERED	2	Staggered corrector forward sensitivity method.
CV_STAGGERED1	3	Staggered (variant) corrector forward sensitivity method.
CV_CENTERED	1	Central difference quotient approximation (2^{nd} order) of the sensitivity RHS.
CV_FORWARD	2	Forward difference quotient approximation (1^{st} order) of the sensitivity RHS.

CVODES **adjoint solver module**		
CV_HERMITE	1	Use Hermite interpolation.
CV_POLYNOMIAL	2	Use variable-degree polynomial interpolation.

Iterative linear solver modules		
PREC_NONE	0	No preconditioning
PREC_LEFT	1	Preconditioning on the left only.
PREC_RIGHT	2	Preconditioning on the right only.
PREC_BOTH	3	Preconditioning on both the left and the right.
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

B.2 CVODES output constants

CVODES **main solver module**		
CV_SUCCESS	0	Successful function return.
CV_TSTOP_RETURN	1	CVode succeeded by reaching the specified stopping point.
CV_ROOT_RETURN	2	CVode succeeded and found one or more roots.
CV_WARNING	99	CVode succeeded but an unusual situation occurred.
CV_TOO_MUCH_WORK	-1	The solver took mxstep internal steps but could not reach tout.
CV_TOO_MUCH_ACC	-2	The solver could not satisfy the accuracy demanded by the user for some internal step.
CV_ERR_FAILURE	-3	Error test failures occurred too many times during one internal time step or minimum step size was reached.
CV_CONV_FAILURE	-4	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
CV_LINIT_FAIL	-5	The linear solver's initialization function failed.
CV_LSETUP_FAIL	-6	The linear solver's setup function failed in an unrecoverable manner.
CV_LSOLVE_FAIL	-7	The linear solver's solve function failed in an unrecoverable manner.
CV_RHSFUNC_FAIL	-8	The right-hand side function failed in an unrecoverable manner.
CV_FIRST_RHSFUNC_ERR	-9	The right-hand side function failed at the first call.
CV_REPTD_RHSFUNC_ERR	-10	The right-hand side function had repetead recoverable errors.
CV_UNREC_RHSFUNC_ERR	-11	The right-hand side function had a recoverable error, but no recovery is possible.
CV_RTFUNC_FAIL	-12	The rootfinding function failed in an unrecoverable manner.
CV_NLS_INIT_FAIL	-13	The nonlinear solver's init routine failed.
CV_NLS_SETUP_FAIL	-14	The nonlinear solver's setup routine failed.
CV_CONSTR_FAIL	-15	The inequality constraints were violated and the solver was unable to recover.
CV_MEM_FAIL	-20	A memory allocation failed.
CV_MEM_NULL	-21	The cvode_mem argument was NULL.
CV_ILL_INPUT	-22	One of the function inputs is illegal.
CV_NO_MALLOC	-23	The CVODE memory block was not allocated by a call to CVodeMalloc.
CV_BAD_K	-24	The derivative order k is larger than the order used.
CV_BAD_T	-25	The time t is outside the last step taken.
CV_BAD_DKY	-26	The output derivative vector is NULL.
CV_TOO_CLOSE	-27	The output and initial times are too close to each other.
CV_NO_QUAD	-30	Quadrature integration was not activated.
CV_QRHSFUNC_FAIL	-31	The quadrature right-hand side function failed in an unrecoverable manner.
CV_FIRST_QRHSFUNC_ERR	-32	The quadrature right-hand side function failed at the first call.
CV_REPTD_QRHSFUNC_ERR	-33	The quadrature ight-hand side function had repetead recoverable errors.

CV_UNREC_QRHSFUNC_ERR	-34	The quadrature right-hand side function had a recoverable error, but no recovery is possible.
CV_NO_SENS	-40	Forward sensitivity integration was not activated.
CV_SRHSFUNC_FAIL	-41	The sensitivity right-hand side function failed in an unrecoverable manner.
CV_FIRST_SRHSFUNC_ERR	-42	The sensitivity right-hand side function failed at the first call.
CV_REPTD_SRHSFUNC_ERR	-43	The sensitivity ight-hand side function had repetead recoverable errors.
CV_UNREC_SRHSFUNC_ERR	-44	The sensitivity right-hand side function had a recoverable error, but no recovery is possible.
CV_BAD_IS	-45	The sensitivity index is larger than the number of sensitivities computed.
CV_NO_QUADSENS	-50	Forward sensitivity integration was not activated.
CV_QSRHSFUNC_FAIL	-51	The sensitivity right-hand side function failed in an unrecoverable manner.
CV_FIRST_QSRHSFUNC_ERR	-52	The sensitivity right-hand side function failed at the first call.
CV_REPTD_QSRHSFUNC_ERR	-53	The sensitivity ight-hand side function had repetead recoverable errors.
CV_UNREC_QSRHSFUNC_ERR	-54	The sensitivity right-hand side function had a recoverable error, but no recovery is possible.

CVODES **adjoint solver module**

CV_NO_ADJ	-101	Adjoint module was not initialized.
CV_NO_FWD	-102	The forward integration was not yet performed.
CV_NO_BCK	-103	No backward problem was specified.
CV_BAD_TBO	-104	The final time for the adjoint problem is outside the interval over which the forward problem was solved.
CV_REIFWD_FAIL	-105	Reinitialization of the forward problem failed at the first checkpoint.
CV_FWD_FAIL	-106	An error occurred during the integration of the forward problem.
CV_GETY_BADT	-107	Wrong time in interpolation function.

CVLS **linear solver interface**

CVLS_SUCCESS	0	Successful function return.
CVLS_MEM_NULL	-1	The cvode_mem argument was NULL.
CVLS_LMEM_NULL	-2	The CVLS linear solver has not been initialized.
CVLS_ILL_INPUT	-3	The CVLS solver is not compatible with the current NVECTOR module, or an input value was illegal.
CVLS_MEM_FAIL	-4	A memory allocation request failed.
CVLS_PMEM_NULL	-5	The preconditioner module has not been initialized.
CVLS_JACFUNC_UNRECVR	-6	The Jacobian function failed in an unrecoverable manner.
CVLS_JACFUNC_RECVR	-7	The Jacobian function had a recoverable error.
CVLS_SUNMAT_FAIL	-8	An error occurred with the current SUNMATRIX module.

CVLS_SUNLS_FAIL	-9	An error occurred with the current SUNLINSOL module.
CVLS_NO_ADJ	-101	The combined forward-backward problem has not been initialized.
CVLS_LMEMB_NULL	-102	The linear solver was not initialized for the backward phase.

CVDIAG **linear solver module**

CVDIAG_SUCCESS	0	Successful function return.
CVDIAG_MEM_NULL	-1	The cvode_mem argument was NULL.
CVDIAG_LMEM_NULL	-2	The CVDIAG linear solver has not been initialized.
CVDIAG_ILL_INPUT	-3	The CVDIAG solver is not compatible with the current NVECTOR module.
CVDIAG_MEM_FAIL	-4	A memory allocation request failed.
CVDIAG_INV_FAIL	-5	A diagonal element of the Jacobian was 0.
CVDIAG_RHSFUNC_UNRECVR	-6	The right-hand side function failed in an unrecoverable manner.
CVDIAG_RHSFUNC_RECVR	-7	The right-hand side function had a recoverable error.
CVDIAG_NO_ADJ	-101	The combined forward-backward problem has not been initialized.

Appendix C

SUNDIALS Release History

Table C.1: Release History

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
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
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

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Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
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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