

User Documentation for CVODE v5.2.0
(SUNDIALS v5.2.0)

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Chapter 1

Introduction

CVODE is part of a software family called SUNDIALS: SUite of Nonlinear and Differential/ALgebraic equation Solvers [29]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities.

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 [40]. 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 conjunction with Newton iteration: these include the GMRES (Generalized Minimal RESidual) [43], FGMRES (Flexible Generalized Minimum RESidual) [42], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [44], TFQMR (Transpose-Free Quasi-Minimal Residual) [22], and PCG (Preconditioned Conjugate Gradient) [24] 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 multiprocessor environments with minimal impacts on the rest of the solver, resulting in PVOE [14], the parallel variant of CVODE.

Around 2002, the functionality of `CVODE` and `PVODE` were combined into one single code, simply called `CVODE`. Development of this version of `CVODE` 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 kernels 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 linked into an executable file. SUNDIALS (and thus `CVODE`) is supplied with six different `NVECTOR` implementations: serial, MPI-parallel, and both OpenMP and Pthreads thread-parallel `NVECTOR` implementations, a Hypré parallel implementation, and a PETSc implementation.

There are several motivations for choosing the C language for `CVODE`. First, a general movement away from FORTRAN and toward C in scientific computing was apparent. Second, the pointer, structure, and dynamic memory allocation features in C are extremely useful in software of this complexity, with the great variety of method options offered. Finally, we prefer C over C++ for `CVODE` 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 v5.2.0

Fixed a build system bug related to the Fortran 2003 interfaces when using the IBM XL compiler. When building the Fortran 2003 interfaces with an XL compiler it is recommended to set `CMAKE_Fortran_COMPILER` to `f2003`, `xlF2003`, or `xlF2003_r`.

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

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

The function `CVodeSetLinearSolutionScaling` was added to enable or disable the scaling applied to linear system solutions with matrix-based linear solvers to account for a lagged value of γ in the linear system matrix $I - \gamma J$. Scaling is enabled by default when using a matrix-based linear solver with BDF methods.

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 9.4.1 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 §6.1.5 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 §6.13 and §6.14 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 §6.1.4 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 §6.15 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 §6.9.1 for more details.
- Added new Fortran 2003 interfaces for most `NVECTOR` modules. See Chapter 6 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 §6.1.5 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 §7.1.2 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 §7.1.1 for more details.
- The generic `SUNMATRIX` API now defines error codes to be returned by `SUNMATRIX` operations. Operations which return an integer flag indicating success/failure may return different values than previously. See §7.1.3 for more details.
- A new `SUNMATRIX` (and `SUNLINSOL`) implementation was added to facilitate the use of the `SuperLU_DIST` library with `SUNDIALS`. See §7.6 for more details.
- Added new Fortran 2003 interfaces for most `SUNMATRIX` modules. See Chapter 7 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 §8.3 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 §8.10 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 §8.12 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 §8.9.2 for more details.
- Added new Fortran 2003 interfaces for most SUNLINSOL modules. See Chapter 8 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 §9.1.8 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 §9.2 and for more details on the API functions see Chapter 9.
- Added a new SUNNONLINSOL implementation, `SUNNONLINSOL_PETSCSNES`, which interfaces to the PETSc SNES nonlinear solver API. See §9.5 for more details.
- Added new Fortran 2003 interfaces for most SUNNONLINSOL modules. See Chapter 9 for more details on how to use the interfaces.

CVODE changes

- Fixed a bug in the CVODE constraint handling where the step size could be set below the minimum step size.
- Fixed a bug in the CVODE nonlinear solver interface where the norm of the accumulated correction was not updated when using a non-default convergence test function.
- Fixed a memory leak in FCVODE when not using the default nonlinear solver.

- Removed extraneous calls to `N_VMin` for simulations where the scalar valued absolute tolerance, or all entries of the vector-valued absolute tolerance array, are strictly positive. In this scenario, `CVODE` 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 two new functions, `CVodeGetCurrentGamma` and `CVodeGetCurrentState`, which may be useful to users who choose to provide their own nonlinear solver implementations.
- The `CVODE` Fortran 2003 interface was completely redone to be more sustainable and to allow users to write more idiomatic Fortran. See Chapter 5 for more details.

Changes in v4.1.0

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

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

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

The implementation header file `cvode_impl.h` is no longer installed. This means users who are directly manipulating the `CVodeMem` structure will need to update their code to use `CVODE`'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 `CVODE` library, `libsundials_cvode`.

Changes in v4.0.1

No changes were made in this release.

Changes in v4.0.0

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

The names of all constructor routines for SUNDIALS-provided SUNLINSOL implementations have been updated to follow the naming convention `SUNLinSol_*` where `*` is the name of the linear solver. The new names are `SUNLinSol_Band`, `SUNLinSol_Dense`, `SUNLinSol_KLU`, `SUNLinSol_LapackBand`, `SUNLinSol_LapackDense`, `SUNLinSol_PCG`, `SUNLinSol_SPBCGS`, `SUNLinSol_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 CVOID example programs and the standalone linear solver examples have been updated to use the new naming convention.

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

SUNDIALS integrators have been updated to utilize generic nonlinear solver modules defined through the `SUNNONLINSOL` API. This API will ease the addition of new nonlinear solver options and allow for external or user-supplied nonlinear solvers. The `SUNNONLINSOL` API and SUNDIALS provided modules are described in Chapter 9 and follow the same object oriented design and implementation used by the `NVECTOR`, `SUNMATRIX`, and `SUNLINSOL` modules. Currently two `SUNNONLINSOL` implementations are provided, `SUNNONLINSOL_NEWTON` and `SUNNONLINSOL_FIXEDPOINT`. These replicate the previous integrator specific implementations of a Newton iteration and a fixed-point iteration (previously referred to as a functional iteration), respectively. Note the `SUNNONLINSOL_FIXEDPOINT` module can optionally utilize Anderson’s method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all CVOID 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`. Similarly, the `ITMETH` parameter has been removed from the Fortran interface function `FCVMALLOC`. Instead of specifying the nonlinear iteration type when creating the CVOID memory structure, CVOID 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 Chapter 4. CVOID 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 6 for more details). The new operations are intended to increase data reuse in vector operations, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. The fused operations are `N_VLinearCombination`, `N_VScaleAddMulti`, and `N_VDotProdMulti` and the vector array operations are `N_VLinearCombinationVectorArray`, `N_VScaleVectorArray`, `N_VConstVectorArray`, `N_VWrmsNormVectorArray`, `N_VWrmsNormMaskVectorArray`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. If an `NVECTOR` implementation defines any of these operations as `NULL`, then standard `NVECTOR` operations will automatically be called as necessary to complete the computation.

Multiple updates to `NVECTOR_CUDA` were made:

- Changed `N_VGetLength_Cuda` to return the global vector length instead of the local vector length.
- Added `N_VGetLocalLength_Cuda` to return the local vector length.
- Added `N_VGetMPIComm_Cuda` to return the MPI communicator used.
- Removed the accessor functions in the namespace `suncudavec`.
- Changed the `N_VMake_Cuda` function to take a host data pointer and a device data pointer instead of an `N_VectorContent_Cuda` object.

- Added the ability to set the `cudaStream_t` used for execution of the `NVECTOR_CUDA` kernels. See the function `N_VSetCudaStreams_Cuda`.
- Added `N_VNewManaged_Cuda`, `N_VMakeManaged_Cuda`, and `N_VIsManagedMemory_Cuda` functions to accommodate using managed memory with the `NVECTOR_CUDA`.

Multiple changes to `NVECTOR_RAJA` were made:

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

A new `NVECTOR` implementation for leveraging OpenMP 4.5+ device offloading has been added, `NVECTOR_OPENMPDEV`. See §6.11 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.

A FORTRAN 2003 interface to `CVODE` has been added along with FORTRAN 2003 interfaces to the following shared SUNDIALS modules:

- `SUNNONLINSOL_FIXEDPOINT` and `SUNNONLINSOL_NEWTON` nonlinear solver modules
- `SUNLINSOL_DENSE`, `SUNLINSOL_BAND`, `SUNLINSOL_KLU`, `SUNLINSOL_PCG`, `SUNLINSOL_SPBCGS`, `SUNLINSOL_SPGMR`, `SUNLINSOL_SPGMR`, and `SUNLINSOL_SPTFQMR` linear solver modules
- `NVECTOR_SERIAL`, `NVECTOR_PTHREADS`, and `NVECTOR_OPENMP` vector modules

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 be 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 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 deprecated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPI_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.
- When a Fortran name-mangling scheme is needed (e.g., `LAPACK_ENABLE` is ON) the build system will infer the scheme from the Fortran compiler. If a Fortran compiler is not available or the inferred or default scheme needs to be overridden, the advanced options `SUNDIALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` can be used to manually set the name-mangling scheme and bypass trying to infer the scheme.
- Parts of the main `CMakeLists.txt` file were moved to new files in the `src` and `example` directories to make the CMake configuration file structure more modular.

Changes in v3.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using `rpath` by default to locate shared libraries on OSX.
- Fixed Windows specific problem where `sunindextype` was not correctly defined when using 64-bit integers for the `SUNDIALS` index type. On Windows `sunindextype` is now defined as the MSVC basic type `__int64`.
- Added sparse SUNMatrix “Reallocate” routine to allow specification of the nonzero storage.
- Updated the KLU SUNLinearSolver module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.
- Updated the “ScaleAdd” and “ScaleAddI” implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum $I + \gamma J$ manually (with zero entries if needed).
- Added the following examples from the usage notes page of the SUNDIALS website, and updated them to work with SUNDIALS 3.x:

- `cvDisc_dns.c`, which demonstrates using CVODE with discontinuous solutions or RHS.
 - `cvRoberts_dns_negsol.c`, which illustrates the use of the RHS function return value to control unphysical negative concentrations.
- 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.
- Fixed compilation issue with GCC 7.3.0 and Fortran programs that do not require a SUNMATRIX or SUNLINSOL module (e.g., iterative linear solvers or fixed-point iteration).

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 the web site, <https://software.llnl.gov/RAJA/>. These additions are accompanied by additions to various interface functions and to user documentation.

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

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

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

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

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.

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

In FCVODE, corrections were made to three Fortran interface functions. Missing Fortran interface routines were added so that users can supply the sparse Jacobian routine when using sparse direct solvers.

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

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

New examples were added for use of the OpenMP vector and for use of sparse direct solvers from Fortran.

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

Changes in v2.8.0

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

Otherwise, only relatively minor modifications were made to the CVODE 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+m1)` was changed to `smu = mu + m1` to correct an illegal input error for `DGBTRF/DGBTRS`.

In order to eliminate or minimize the differences between the sources for private functions in CVODE and CVODES, the names of 48 private functions were changed from `CV**` to `cv**`, and a few other names were also changed.

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`.

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

The example program `cvAdvDiff_diag_p` was added to illustrate the use of `CVDiag` in parallel.

In the FCVODE optional input routines `FCVSETIIN` and `FCVSETRIN`, the optional fourth argument `key_length` was removed, with hardcoded key string lengths passed to all `strncmp` tests.

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

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

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

Changes in v2.7.0

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

A large number of minor errors have been fixed. Among these are the following: 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 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.

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.

Changes in v2.5.0

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

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). Corresponding additions were made to the FORTRAN interface module `FCVODE`. At the same time, function type names for Scaled Preconditioned Iterative Linear Solvers were added for the user-supplied Jacobian-times-vector and preconditioner setup and solve functions.

The 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 (`cvode_` and `sundials_`). When using the default installation procedure, the header

files are exported under various subdirectories of the target `include` directory. For more details see Appendix A.

Changes in v2.3.0

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

Changes in v2.2.1

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

Changes in v2.2.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the `iopt` and `ropt` arrays. Instead, CVODE 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 and preconditioner information) were simplified by reducing the number of arguments. The same information that was previously accessible through such arguments can now be obtained through `Get`-type functions.

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 CVODE (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 CVODE. 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 [31].

In a different direction, a more expert user with an IVP problem may want to (a) use a package preconditioner (§4.7), (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 6), (e) supply new SUNLINSOL and/or SUNMATRIX modules (Chapters 7 and 8), or even (f) supply new SUNNONLINSOL modules (Chapter 9).

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by CVODE for the solution of initial value problems for systems of ODEs, and continue with short descriptions of preconditioning (§2.2), stability limit detection (§2.3), and rootfinding (§2.4).
- The following chapter describes the structure of the SUNDIALS suite of solvers (§3.1) and the software organization of the CVODE solver (§3.2).

- Chapter 4 is the main usage document for CVODE for C applications. It includes a complete description of the user interface for the integration of ODE initial value problems.
- In Chapter 5, we describe the use of CVODE with FORTRAN applications.
- Chapter 6 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 7 gives a brief overview of the generic SUNMATRIX module shared among the various components of SUNDIALS, and details on the SUNMATRIX implementations provided with SUNDIALS: a dense implementation (§7.3), a banded implementation (§7.4) and a sparse implementation (§7.5).
- Chapter 8 gives a brief overview of the generic SUNLINSOL module shared among the various components of SUNDIALS. This chapter contains details on the SUNLINSOL implementations provided with SUNDIALS. The chapter also contains details on the SUNLINSOL implementations provided with SUNDIALS that interface with external linear solver libraries.
- Chapter 9 describes the SUNNONLINSOL API and nonlinear solver implementations shared among the various components of SUNDIALS.
- Finally, in the appendices, we provide detailed instructions for the installation of CVODE, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from CVODE 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 CVLS, are written in all capitals. Usage and installation instructions that constitute important warnings are marked with a triangular symbol in the margin.



Acknowledgments. We wish to acknowledge the contributions to previous versions of the CVODE and PVODE codes and their user guides by Scott D. Cohen [15] and George D. Byrne [13].

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1.4.3 SUNDIALS Release Numbers

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LLNL-CODE-665877 (KINSOL)

Chapter 2

Mathematical Considerations

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

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

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. CVODE 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.

2.1 IVP solution

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

$$\sum_{i=0}^{K_1} \alpha_{n,i} y^{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{y}^{n-i} = 0. \quad (2.2)$$

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, CVODE 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 [33].

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

$$F(y^n) \equiv y^n - h_n \beta_{n,0} f(t_n, y^n) - a_n = 0, \quad (2.3)$$

or as a fixed-point problem

$$G(y^n) \equiv h_n \beta_{n,0} f(t_n, y^n) + a_n = y^n. \quad (2.4)$$

where $a_n \equiv \sum_{i>0} (\alpha_{n,i} y^{n-i} + h_n \beta_{n,i} \dot{y}^{n-i})$. CVODE provides several nonlinear solver choices as well as the option of using a user-defined nonlinear solver (see Chapter 9). By default CVODE solves (2.3) with a *Newton iteration* which requires the solution of linear systems

$$M[y^{n(m+1)} - y^{n(m)}] = -F(y^{n(m)}), \quad (2.5)$$

in which

$$M \approx I - \gamma J, \quad J = \partial f / \partial y, \quad \text{and} \quad \gamma = h_n \beta_{n,0}. \quad (2.6)$$

The exact variation of the Newton iteration depends on the choice of linear solver and is discussed below and in §9.3. For nonstiff systems, a *fixed-point iteration* (previously referred to as a functional

iteration in this guide) solving (2.4) is also available. This involves evaluations of f only and can (optionally) use Anderson’s method [5, 45, 21, 39] to accelerate convergence (see §9.4 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 (2.5) (e.g., the default Newton iteration), CVODE provides several linear solver choices, including the option of a user-supplied linear solver module (see Chapter 8). The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices, and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- band direct solvers, using either an internal implementation or a BLAS/LAPACK implementation (serial or threaded vector modules only),
- sparse direct solver interfaces, using either the KLU sparse solver library [17, 1], or the thread-enabled SuperLU_MT sparse solver library [36, 19, 4] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of CVODE],
- 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, CVODE 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

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

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

In the case of a matrix-based linear solver, the default Newton iteration is a Modified Newton iteration, in that the 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 (2.3), 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 (2.7). 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

$$Jv = [f(t, y + \sigma v) - f(t, y)]/\sigma. \quad (2.8)$$

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

A critical part of CVODE — 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 $\|\text{LTE}\| \leq 1$. 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

$$\|\Delta_n\| \leq \epsilon \equiv 1/|C'|.$$

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, CVODE 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, $\text{LTE}(q')$, behaves asymptotically as $h^{q'+1}$. With safety factors of $1/6$ and $1/10$ respectively, these ratios are:

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

and

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

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 CVODE described above, as inherited from VODE and VODPK, are documented in [8, 11, 28]. They are also summarized in [29].

CVODE 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, CVODE estimates a new step size h' using a linear approximation of the components in y that failed the constraint test (including a safety factor of 0.9 to cover the strict inequality case). 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, CVODE takes steps until a user-defined output value $t = t_{\text{out}}$ is overtaken, and then it computes $y(t_{\text{out}})$ by interpolation. However, a “one step” mode option is available, where control returns to the calling program after each step. There are also options to force CVODE not to integrate past a given stopping point $t = t_{\text{stop}}$.

2.2 Preconditioning

When using a nonlinear solver that requires the solution of the linear system (2.5) (e.g., the default Newton iteration), CVODE 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 $P_L P_R$ 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 CVODE 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 Krylov iteration occurs within a nonlinear solver iteration and further also within a time integration, and since each of these iterations has its own test for convergence, the preconditioner may use a very crude approximation, as long as it captures the dominant numerical feature(s) of the system. We have found that the combination

of a preconditioner with the Newton-Krylov iteration, using even a fairly poor approximation to the Jacobian, can be surprisingly superior to using the same matrix without Krylov acceleration (i.e., a modified Newton iteration), as well as to using the Newton-Krylov method with no preconditioning.

2.3 BDF stability limit detection

CVODE 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 [26]. 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 CVODE. 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 [27], where it works well. The implementation in CVODE 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 CVODE solver has been augmented to include a rootfinding feature. This means that, while integrating the Initial Value Problem (2.1), CVODE 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 CVODE. 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 [25]. In addition, each time g is computed, CVODE 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 , CVODE 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, CVODE stops and reports an error. This way, each time CVODE 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, CVODE 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 $\tau/2$.

Chapter 3

Code Organization

3.1 SUNDIALS organization

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

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

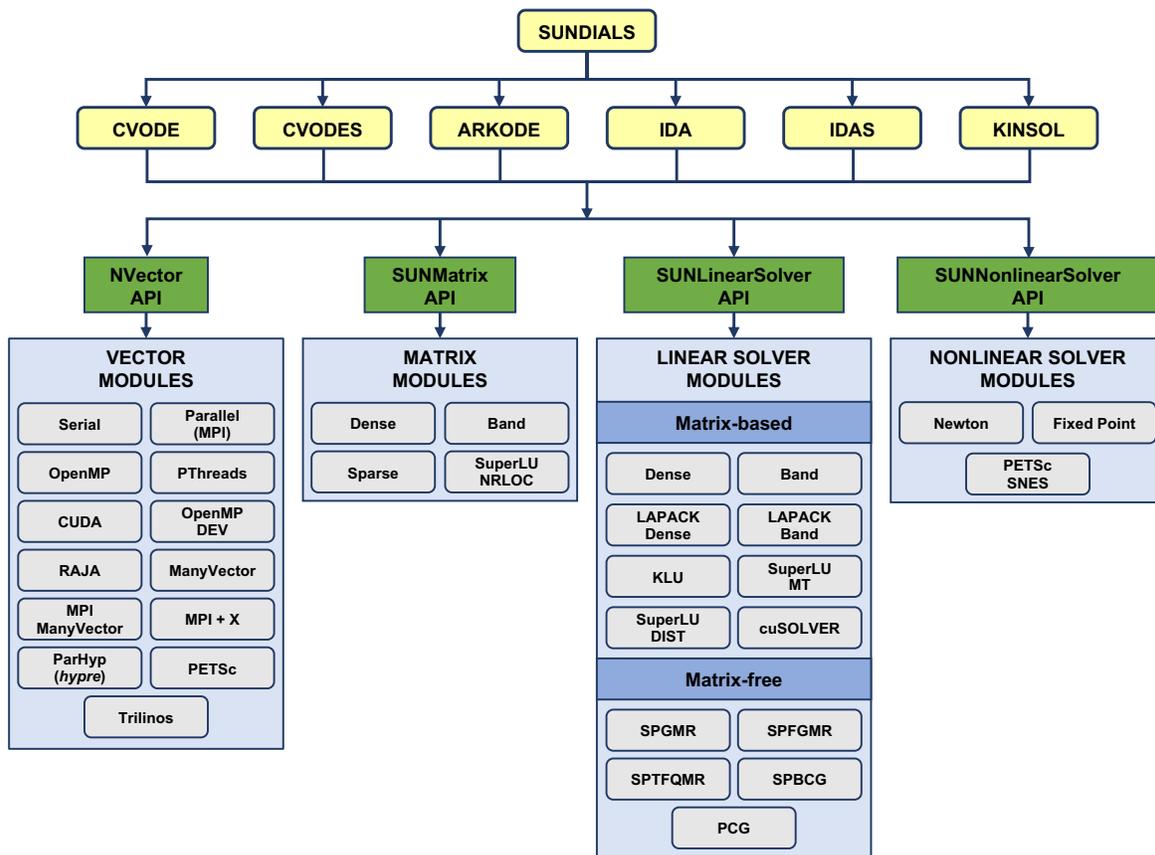


Figure 3.1: High-level diagram of the SUNDIALS suite.

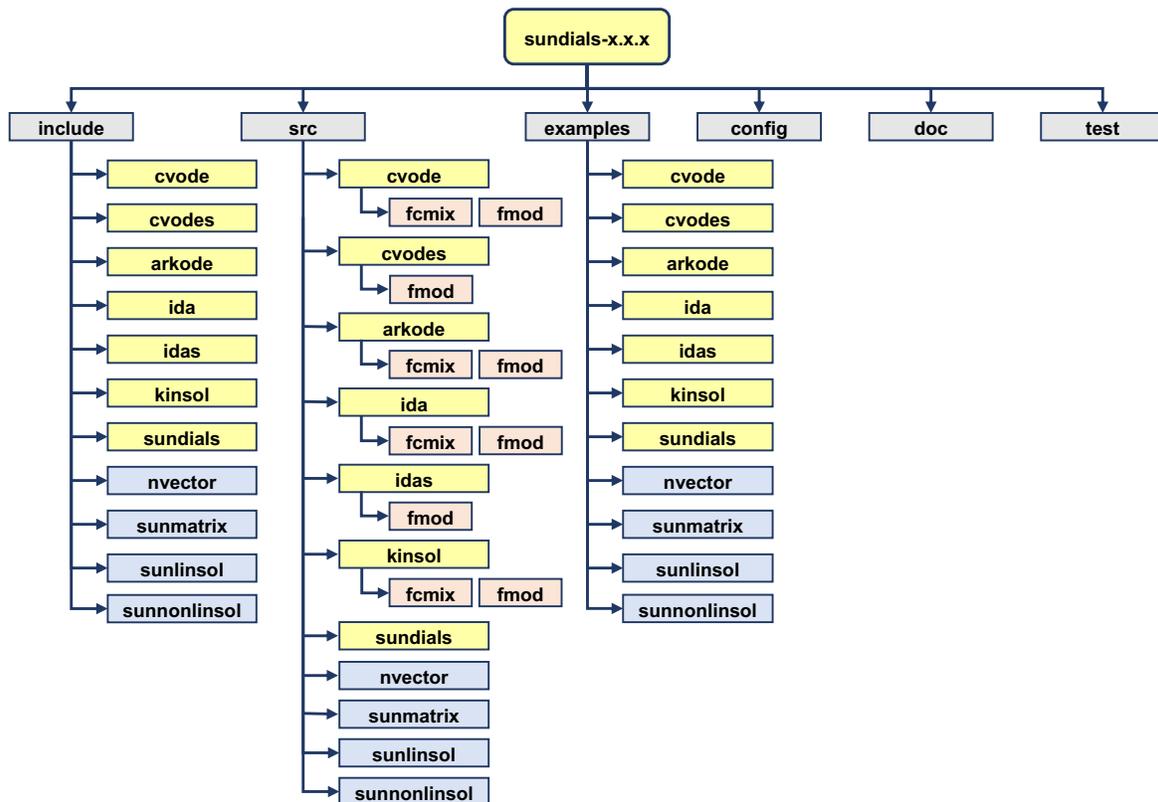


Figure 3.2: Directory structure of the SUNDIALS source tree.

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

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

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

3.2 CVODE organization

The CVODE 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 CVODE package is shown in Figure 3.3. The central integration module, implemented in the files `cvode.h`, `cvode_impl.h`, and `cvode.c`, deals with the evaluation of

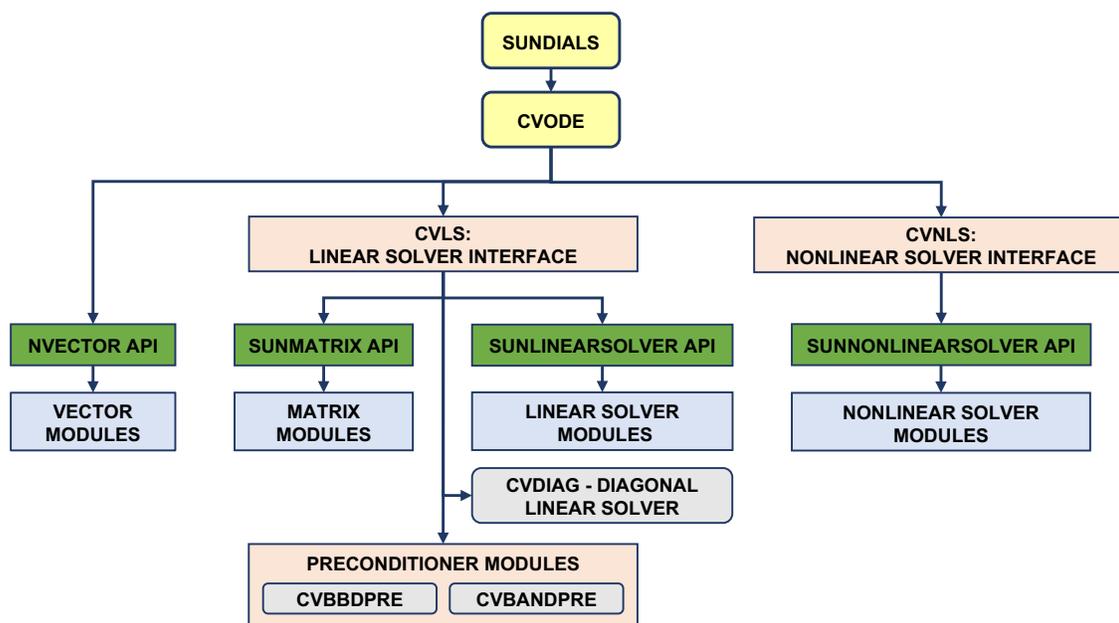


Figure 3.3: Overall structure diagram of the CVODE package. Modules specific to CVODE begin with “CV” (CVLS, CVNLS, CVDIAG, CVBBDPRE, and CVBANDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver modules (see Figure 3.1).

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

CVODE utilizes generic linear and nonlinear solver modules defined by the SUNLINSOL API (see Chapter 8) and SUNNONLINSOL API (see Chapter 9) respectively. As such, CVODE 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.

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 8). These solvers may utilize a SUNMATRIX object (see Chapter 7) for storing Jacobian information, or they may be matrix-free. Since CVODE can operate on any valid SUNLINSOL implementation, the set of linear solver modules available to CVODE will expand as new SUNLINSOL modules are developed.

Additionally, CVODE includes the *diagonal* linear solver interface, CVDIAG, that creates an internally generated diagonal approximation to the Jacobian.

For users employing dense or banded Jacobian matrices, CVODE 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, CVODE 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 CVODE, offer considerable assistance in building preconditioners.

CVODE’s 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.

CVODE 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 CVODE 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 CVODE 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 CVODE memory structure. The reentrancy of CVODE 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 CVODE for C Applications

This chapter is concerned with the use of CVODE 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 CVODE user-callable functions and user-supplied functions.

The sample programs described in the companion document [31] 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 CVODE package.

Users with applications written in FORTRAN should see Chapter 5, which describes interfacing with CVODE from FORTRAN.

The user should be aware that not all SUNLINSOL and SUNMATRIX modules are compatible with all NVECTOR implementations. Details on compatibility are given in the documentation for each SUNMATRIX module (Chapter 7) and each SUNLINSOL module (Chapter 8). For example, NVECTOR_PARALLEL is not compatible with the dense, banded, or sparse SUNMATRIX types, or with the corresponding dense, banded, or sparse SUNLINSOL modules. Please check Chapters 7 and 8 to verify compatibility between these modules. In addition to that documentation, we note that the 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.

CVODE 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 CVODE, 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 CVODE. The relevant library files are

- *libdir/libsundials_cvode.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/cvode*
- *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).

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:

- `cvode/cvode.h`, the main header file for CVODE, which defines the several types and various constants, and includes function prototypes. This includes the header file for CVLS, `cvode/cvode_ls.h`.

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

The calling program must also include an NVECTOR implementation header file, of the form `nvector/nvector_***.h`. See Chapter 6 for the appropriate name. This file in turn includes the header file `sundials_nvector.h` which defines the abstract `N_Vector` data type.

If using a non-default nonlinear solver module, or when interacting with a `SUNNONLINSOL` module directly, the calling program must also include a `SUNNONLINSOL` implementation header file, of the form `sunnonlinsol/sunnonlinsol_***.h` where `***` is the name of the nonlinear solver module (see Chapter 9 for more information). This file in turn includes the header file `sundials_nonlinearsolver.h` which defines the abstract `SUNNonlinearSolver` data type.

If using a nonlinear solver that requires the solution of a linear system of the form (2.5) (*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 CVODE 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_spgfmr.h`, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, `SUNLINSOL_SPGFMR`;
 - `sunlinsol/sunlinsol_spgbcs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, `SUNLINSOL_SPGBCGS`;
 - `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`;
- `cvode/cvode_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 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 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 `cvDiurnal_kry_p` example (see [31]), 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 6, 7, 8, and 9 for the specific name of the function to be called or macro to be referenced.

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

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

2. Set problem dimensions etc.

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

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

3. Set 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 §6.3-6.6 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 §6.7 and §6.8 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 §6.9-6.10 for details.

4. Create CVOICE object

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

5. Initialize CVOICE solver

Call `CVodeInit(...)` to provide required problem specifications, allocate internal memory for CVOICE, and initialize CVOICE. `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 default Newton iteration) and the linear solver will be a matrix-based linear solver, then a template Jacobian matrix must be created by calling the appropriate constructor function defined by the particular SUNMATRIX implementation.

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

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

or

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

or

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

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

8. Create linear solver object

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

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

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

where `*` can be replaced with “Dense”, “SPGMR”, or other options, as discussed in §4.5.3 and Chapter 8.

9. Set linear solver optional inputs

Call `*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See the documentation for each SUNLINSOL module in Chapter 8 for details.

10. Attach linear solver module

If a nonlinear solver requiring a linear solver is chosen (e.g., the default Newton iteration), then initialize the 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 CVODE-specific diagonal linear solver module, CVDIAG, is desired, initialize the linear solver module and attach it to CVODE with the call

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

11. Set optional inputs

Call `CVodeSet*` functions to change any optional inputs that control the behavior of CVODE 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 9 for details).

13. Attach nonlinear solver module (*optional*)

If using a non-default nonlinear solver, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling `ier = 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 CVODE defaults. See Chapter 9 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 `CVODE`.

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 8 the SUNDIALS packages operate on generic `SUNLINSOL` objects, allowing a user to develop their own solvers should they so desire.

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

Linear Solver	Serial	Parallel (MPI)	OpenMP	pThreads	hypr	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 `CVODE` 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 CVODE. 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 CVODE 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 CVODE memory block created and allocated by the first two calls.

CVodeCreate

Call `cvode_mem = CVodeCreate(lmm);`

Description The function `CVodeCreate` instantiates a CVODE 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 CVODE see the description of `CVodeSetNonlinearSolver`.

Return value If successful, `CVodeCreate` returns a pointer to the newly created CVODE 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 CVODE.

Arguments `cvode_mem` (`void *`) pointer to the CVODE 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 CVODE 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 CVODE memory block (of type `void *`).

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

F2003 Name `FCVodeFree`

4.5.2 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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	<code>flag = CVodeWftolerances(cvode_mem, efun);</code>
Description	The function <code>CVodeWftolerances</code> specifies a user-supplied function <code>efun</code> that sets the multiplicative error weights W_i for use in the weighted RMS norm, which are normally defined by Eq. (2.7).
Arguments	<code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block returned by <code>CVodeCreate</code> . <code>efun</code> (<code>CVEwtFn</code>) is the C function which defines the <code>ewt</code> vector (see §4.6.3).
Return value	The return value <code>flag</code> (of type <code>int</code>) will be one of the following: <code>CV_SUCCESS</code> The call to <code>CVodeWftolerances</code> was successful. <code>CV_MEM_NULL</code> The CVODE memory block was not initialized through a previous call to <code>CVodeCreate</code> . <code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> 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 `cvRoberts_dns` in the CVODE package, and the discussion of it in the CVODE Examples document [31]. In that problem, the three components vary between 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

(3) Finally, it is important to pick all the tolerance values conservatively, because they control the error committed on each individual time step. The final (global) errors are 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 CVODE, 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 (2.5) (e.g., the default Newton iteration), there are two CVODE linear solver interfaces currently available for this task: CVLS and CVDIAG.

The first corresponds to the main linear solver interface in CVODE, 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 (2.6).

The CVDIAG linear solver interface supports a direct linear solver, that uses only a diagonal approximation to J .

To specify a generic linear solver to CVODE, after the call to `CVodeCreate` but before any calls to `CVode`, 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 7 and 8.

Once this solver object has been constructed, the user should attach it to CVODE via a call to `CVodeSetLinearSolver`. The first argument passed to this function is the CVODE 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 CVODE integrator, and allows the user to specify additional parameters and routines pertinent to their choice of linear solver.

To instead specify the CVODE-specific diagonal linear solver interface, the user's program must call `CVDiag`, as documented below. The first argument passed to this function is the CVODE 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` (if applicable) to CVODE, initializing the CVLS linear solver interface.
- Arguments `cvode_mem` (`void *`) pointer to the CVODE memory block.
`LS` (`SUNLinearSolver`) SUNLINSOL object to use for solving linear systems of the form (2.5).
`J` (`SUNMatrix`) SUNMATRIX object for used as a template for the Jacobian (or NULL if not applicable).
- Return value The return value `flag` (of type `int`) is one of
`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 7 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 `cvode_diag.h` header file.
- Arguments `cvode_mem` (`void *`) pointer to the CVODE 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 CVODE linear solvers. 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 `CVODE` uses the `SUNNONLINSOL` implementation of Newton's method defined by the `SUNNONLINSOL_NEWTON` module (see §9.3). To specify a different nonlinear solver in `CVODE`, 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 `CVODE`, `CVodeSetNonlinearSolver` must be called after `CVodeInit`. If any calls to `CVode` have been made, then `CVODE` 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 `CVODE` memory pointer returned by `CVodeCreate` and the second argument is the `SUNNONLINSOL` object to use for solving the nonlinear system (2.3) or (2.4). A call to this function attaches the nonlinear solver to the main `CVODE` integrator.

`CVodeSetNonlinearSolver`

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

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

Arguments `cvode_mem` (`void *`) pointer to the `CVODE` memory block.
`NLS` (`SUNNonlinearSolver`) `SUNNONLINSOL` object to use for solving nonlinear systems (2.3) or (2.4).

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 FCVodeSetNonlinearSolver

4.5.5 Rootfinding initialization function

While solving the IVP, `CVODE` 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 `CVODE` 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 CVODE 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 CVODE 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 CVODE 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 $y(\text{tout})$. 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 $t = \text{tret}$, 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 CVODE 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 <code>mxstep</code> internal steps but still could not reach <code>tout</code> . The default value for <code>mxstep</code> is <code>MXSTEP_DEFAULT = 500</code> .
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 (<code>MXNEF = 7</code>) during one internal time step, or with $ h = h_{min}$.
CV_CONV_FAILURE	Either convergence test failures occurred too many times (<code>MXNCF = 10</code>) 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 through 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`

4.5.7 Optional input functions

There are numerous optional input parameters that control the behavior of the `CVODE` solver. `CVODE` provides functions that can be used to change these optional input parameters from their default

Table 4.2: Optional inputs for CVODE and CVLS

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

values. Table 4.2 lists all optional input functions in CVODE which are then described in detail in the remainder of this section, beginning with those for the main CVODE 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 CVODE, 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 CVODE messages should be directed when the default CVODE error handler function is used.

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

`ehfun` (`CErrorHandlerFn`) 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 `CVODE` 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 `CVODE` memory block.

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

`stldet` (boolean type) 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 CVODE 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, CVODE 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 t_0 .

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 CVODE 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 CVODE 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 CVODE 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 through 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 CVODE 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 CVODE 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 `CVODE` 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 `CVODE` 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`

`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 `CVODE` memory block.
`constraints` (`N_Vector`) vector of constraint flags. If `constraints[i]` is
0.0 then no constraint is imposed on y_i .
1.0 then y_i will be constrained to be $y_i \geq 0.0$.
-1.0 then y_i will be constrained to be $y_i \leq 0.0$.
2.0 then y_i will be constrained to be $y_i > 0.0$.
-2.0 then y_i will be constrained to be $y_i < 0.0$.

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

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.

F2003 Name `FCVodeSetConstraints`

4.5.7.2 Linear solver interface optional input functions

The mathematical explanation of the linear solver methods available to CVODE 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, CVODE 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, CVODE 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`.

<code>CVodeSetMaxStepsBetweenJac</code>

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 CVODE 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 CVODE 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 CVODE 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 a matrix-based linear solver the matrix information will be updated infrequently to reduce matrix construction and, with direct solvers, factorization costs. As a result the value of γ may not be current and, with BDF methods, a scaling factor is applied to the solution of the linear system to account for the lagged value of γ . See §8.4.1 for more details. The function `CVodeSetLinearSolutionScaling` can be used to disable this scaling when necessary, e.g., when providing a custom linear solver that updates the matrix using the current γ as part of the solve.

CVodeSetLinearSolutionScaling

Call `flag = CVodeSetLinearSolutionScaling(cvode_mem, onoff);`

Description The function `CVodeSetLinearSolutionScaling` enables or disables scaling the linear system solution to account for a change in γ in the linear system. For more details see §8.4.1.

Arguments `cvode_mem` (`void *`) pointer to the CVODE memory block.
`onoff` (`booleantype`) flag to enable (`SUNTRUE`) or disable (`SUNFALSE`) scaling

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

- `CVLS_SUCCESS` The flag 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.
- `CVLS_ILL_INPUT` The attached linear solver is not matrix-based or the linear multistep method type is not BDF.

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

By default scaling is enabled with matrix-based linear solvers when using BDF methods.

F2003 Name FCVodeSetLinearSolutionScaling

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 CVODE 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 `jt看imes` and to omit `jtsetup`. If NULL is passed to `jt看imes`, these defaults are used. A user may specify non-NULL `jt看imes` 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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	<code>flag = CVodeSetNoInactiveRootWarn(cvode_mem);</code>
Description	The function <code>CVodeSetNoInactiveRootWarn</code> disables issuing a warning if some root function appears to be identically zero at the beginning of the integration.
Arguments	<code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block.
Return value	The return value <code>flag</code> (of type <code>int</code>) is one of <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .
Notes	CVODE 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), CVODE will issue a warning which can be disabled with this optional function.
F2003 Name	<code>FCVodeSetNoInactiveRootWarn</code>

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 CVODE.

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

CVodeGetDky

Call	<code>flag = CVodeGetDky(cvode_mem, t, k, dky);</code>
Description	The function <code>CVodeGetDky</code> computes the k -th derivative of the function y at time t , i.e. $d^{(k)}y/dt^{(k)}(t)$, where $t_n - h_u \leq t \leq t_n$, 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 $k = 0, 1, \dots, q_u$, where q_u is the current order (optional output <code>qlast</code>).
Arguments	<code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block. t (<code>realtype</code>) the value of the independent variable at which the derivative is to be evaluated. k (<code>int</code>) the derivative order requested. <code>dky</code> (<code>N_Vector</code>) vector containing the derivative. This vector must be allocated by the user.
Return value	The return value <code>flag</code> (of type <code>int</code>) is one of <code>CV_SUCCESS</code> <code>CVodeGetDky</code> succeeded. <code>CV_BAD_K</code> k is not in the range $0, 1, \dots, q_u$. <code>CV_BAD_T</code> t is not in the interval $[t_n - h_u, t_n]$. <code>CV_BAD_DKY</code> The <code>dky</code> argument was <code>NULL</code> . <code>CV_MEM_NULL</code> The <code>cvode_mem</code> argument was <code>NULL</code> .
Notes	It is only legal to call the function <code>CVodeGetDky</code> after a successful return from <code>CVode</code> . See <code>CVodeGetCurrentTime</code> , <code>CVodeGetLastOrder</code> , and <code>CVodeGetLastStep</code> in the next section for access to t_n , q_u , and h_u , respectively.
F2003 Name	<code>FCVodeGetDky</code>

4.5.9 Optional output functions

CVODE provides an extensive set of functions that can be used to obtain solver performance information. Table 4.3 lists all optional output functions in CVODE, 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 CVODE 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 `nmiters/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/nmiters` (in the case of a matrix-based linear solver), and the ratio `npevals/nmiters` (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/nmiters` 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/nmiters` 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 CVODE, CVLS, and CVDIAG

Optional output	Function name
CVODE main solver	
Size of CVODE 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 CVODE integrator statistics	CVodeGetIntegratorStats
CVODE 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	CVodeGetLinWorkSpace
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

CVODE 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 CVODE 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 CVODE 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 CVODE real and integer workspace sizes.

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

`lenrw` (`long int`) the number of `realtyp`e values in the CVODE workspace.

`leniw` (`long int`) the number of integer values in the CVODE 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 `realtyp`e words, is given by the following:

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

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) * Ni + nrtfn`;
- using `CVodeSVtolerances`: `leniw = leniw + Ni`;
- with constraint checking: `leniw = leniw + Ni`;

where N_i is the number of integer words in one `N_Vector` (= 1 for `NVECTOR_SERIAL` and $2 * \text{nps}$ for `NVECTOR_PARALLEL` and `nps` 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`

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 CVODE memory block.

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

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 `cvoid_mem` pointer is NULL.

F2003 Name `FCVodeGetNumSteps`

`CVodeGetNumRhsEvals`

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

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

Arguments `cvoid_mem` (`void *`) pointer to the CVODE 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 `cvoid_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(cvoid_mem, &nlinsetups);`

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

Arguments `cvoid_mem` (`void *`) pointer to the CVODE 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 `cvoid_mem` pointer is NULL.

F2003 Name `FCVodeGetNumLinSolvSetups`

`CVodeGetNumErrTestFails`

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

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

Arguments `cvoid_mem` (`void *`) pointer to the CVODE 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 `cvoid_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 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVODE to ensure that the step size is within the prescribed bounds ($h_{\min} \leq h_0 \leq h_{\max}$), or to satisfy the local error test condition.

F2003 Name `FCVodeGetActualInitStep`

CVodeGetCurrentTime

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

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

Arguments `cvode_mem` (`void *`) pointer to the CVODE memory block.
`tcurl` (`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, &nsred);`

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 CVODE memory block.
`nsred` (`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 `nsred = 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 CVODE 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 (2.7).

Arguments `cvode_mem` (`void *`) pointer to the CVODE 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 CVODE 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, together 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, &tcu);`

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

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

nsteps (long int) number of steps taken by CVODE.
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 CVODE 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 CVODE 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 CVODE nonlinear solver statistics as a group.

Arguments **cvode_mem** (void *) pointer to the CVODE 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 CVODE constant corresponding to `flag`.

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

`rootsfound` (`int *`) array of length `nrtfn` with the indices of the user functions g_i found to have a root. For $i = 0, \dots, nrtfn-1$, `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 CVODE 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 CVOID 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 CVOID 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVODE 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 CVOICE 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 `CVodeGetLastLinFlag` returns the last return value from a CVLS routine.

Arguments `cvode_mem` (`void *`) pointer to the CVOICE 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 $1 \leq \text{lsflag} \leq N$ (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 CVODE memory block.

`lenrwLS` (`long int`) the number of `realtyp`e 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 values 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 $3N$ `realtyp`e 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 CVODE 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 `CVODE` 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 CVODE reinitialization function

The function `CVodeReInit` reinitializes the main `CVODE` 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 extension 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 CVODE.

Arguments `cvode_mem` (`void *`) pointer to the CVODE 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 CVODE memory block was not initialized through a previous call to `CVodeCreate`.

`CV_NO_MALLOC` Memory space for the CVODE 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	<p><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the dependent variable vector, $y(t)$.</p> <p><code>ydot</code> is the output vector $f(t, y)$.</p> <p><code>user_data</code> is the <code>user_data</code> pointer passed to <code>CVodeSetUserData</code>.</p>
Return value	A <code>CVRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODE</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_RHSFUNC_FAIL</code> is returned).
Notes	<p>Allocation of memory for <code>ydot</code> is handled within <code>CVODE</code>.</p> <p>A recoverable failure error return from the <code>CVRhsFn</code> is typically used to flag a value of the dependent variable <code>y</code> that is “illegal” in some way (e.g., negative where only a non-negative value is physically meaningful). If such a return is made, <code>CVODE</code> will attempt to recover (possibly repeating the nonlinear solve, or reducing the step size) in order to avoid this recoverable error return.</p> <p>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.)</p> <p>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 <code>CVRhsFn</code> (in which case <code>CVODE</code> returns <code>CV_FIRST_RHSFUNC_ERR</code>). The other is when a recoverable error is reported by <code>CVRhsFn</code> after an error test failure, while the linear multistep method order is equal to 1 (in which case <code>CVODE</code> returns <code>CV_UNREC_RHSFUNC_ERR</code>).</p>

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 `CVErrorHandlerFn` to process any such messages. The function type `CVErrorHandlerFn` is defined as follows:

`CVErrorHandlerFn`

Definition

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

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

Arguments `error_code` is the error code.

`module` is the name of the `CVODE` 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 `CVodeSetErrorHandlerFn`.

Return value A `CVErrorHandlerFn` 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. (2.7). The function type `CVEwtFn` is defined as follows:

CVEwtFn	
Definition	<code>typedef int (*CVEwtFn)(N_Vector y, N_Vector ewt, void *user_data);</code>
Purpose	This function computes the WRMS error weights for the vector y .
Arguments	<p>y is the value of the dependent variable vector at which the weight vector is to be computed.</p> <p>ewt is the output vector containing the error weights.</p> <p>$user_data$ is a pointer to user data, the same as the $user_data$ parameter passed to <code>CVodeSetUserData</code>.</p>
Return value	A <code>CVEwtFn</code> function type must return 0 if it successfully set the error weights and -1 otherwise.
Notes	<p>Allocation of memory for ewt is handled within <code>CVODE</code>.</p> <p>The error weight vector must have all components positive. It is the user's responsibility to perform this test and return -1 if it is not satisfied.</p>



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	<code>typedef int (*CVRootFn)(realtype t, N_Vector y, realtype *gout, void *user_data);</code>
Purpose	This function implements a vector-valued function $g(t, y)$ such that the roots of the <code>nrtfn</code> components $g_i(t, y)$ are sought.
Arguments	<p>t is the current value of the independent variable.</p> <p>y is the current value of the dependent variable vector, $y(t)$.</p> <p>$gout$ is the output array, of length <code>nrtfn</code>, with components $g_i(t, y)$.</p> <p>$user_data$ is a pointer to user data, the same as the $user_data$ parameter passed to <code>CVodeSetUserData</code>.</p>
Return value	A <code>CVRootFn</code> should return 0 if successful or a non-zero value if an error occurred (in which case the integration is halted and <code>CVode</code> returns <code>CV_RTFUNC_FAIL</code>).
Notes	Allocation of memory for $gout$ is automatically handled within <code>CVODE</code> .

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 optionally provide a function of type `CVLsJacFn` for evaluating the Jacobian of the ODE right-hand side function (or an approximation of it). `CVLsJacFn` is defined as follows:

CVLsJacFn	
Definition	<code>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);</code>
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 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`).

Notes Information regarding the structure of the specific `SUNMATRIX` structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific `SUNMATRIX` interface functions (see Chapter 7 for details).

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 $i, j = 0 \dots N - 1$). 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) = Jm,n`. Alternatively, `SM_COLUMN_D(J, j)` returns a pointer to the first element of the j -th column of `Jac` (with $j = 0 \dots N - 1$), 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] = Jm,n`. For large problems, it is more efficient to use `SM_COLUMN_D` than to use `SM_ELEMENT_D`. Note that both of these macros number rows and columns starting from 0. The `SUNMATRIX_DENSE` type and accessor macros are documented in §7.3.

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 $-\text{mupper} \leq m-n \leq \text{mlower}$. 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 `realtyp *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 $-\text{mupper}$ to `mlower`. For large problems, it is more efficient to use `SM_COLUMN_B` and `SM_COLUMN_ELEMENT_B` than to use the `SM_ELEMENT_B` macro. As in the dense case, these macros all number rows and columns starting from 0. The `SUNMATRIX_BAND` type and accessor macros are documented in §7.4.

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 §7.5.

The previous function type `CVD1sJacFn` 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:

<code>CVLsLinSysFn</code>

Definition `typedef int (*CVLsLinSysFn)(realtyp t, N_Vector y, N_Vector fy, SUNMatrix M, booleantyp jok, booleantyp *jcur, realtyp 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

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 (\mathbf{t}, \mathbf{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 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, CVODE provides a banded preconditioner in the module `CVBANDPRE` and a band-block-diagonal preconditioner module `CVBBDPRE`.

4.7.1 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 \mathbf{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 `cvode_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 CVODE object
5. Initialize CVODE 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:

<code>CVBandPrecInit</code>

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 CVODE memory block.
`N` (`sunindextype`) problem dimension.
`mu` (`sunindextype`) upper half-bandwidth of the Jacobian approximation.
`m1` (`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 $-m1 \leq j - i \leq mu$.

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 CVODE memory block.
`lenrwBP` (`long int`) the number of `realttype` 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 CVODE 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`

4.7.2 A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel ODE solver such as CVODE lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (2.5) that must be solved at each time step. The linear algebraic system is large, sparse, and structured. However, if a Krylov iterative method is to be effective in this setting, then a nontrivial preconditioner needs to be used. Otherwise, the rate of convergence of the Krylov iterative method is usually unacceptably slow. Unfortunately, an effective preconditioner tends to be problem-specific.

However, we have developed one type of preconditioner that treats a rather broad class of PDE-based problems. It has been successfully used for several realistic, large-scale problems [32] and is included in a software module within the CVODE 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

$$g(t, y) = [g_1(t, \bar{y}_1), g_2(t, \bar{y}_2), \dots, g_M(t, \bar{y}_M)]^T \quad (4.1)$$

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

$$P = \text{diag}[P_1, P_2, \dots, P_M] \quad (4.2)$$

where

$$P_m \approx I - \gamma J_m \quad (4.3)$$

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

$$Px = b \quad (4.4)$$

reduces to solving each of the equations

$$P_m x_m = b_m \quad (4.5)$$

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 `cfm` (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 `cfm`, and that are then used by `gloc`, which should not do any communication.

CVLocalFn

Definition	<code>typedef int (*CVLocalFn)(sunindextype Nlocal, realtype t, N_Vector y, N_Vector glocal, void *user_data);</code>
Purpose	This <code>gloc</code> function computes $g(t, y)$. It loads the vector <code>glocal</code> as a function of <code>t</code> and <code>y</code> .
Arguments	<code>Nlocal</code> is the local vector length. <code>t</code> is the value of the independent variable. <code>y</code> is the dependent variable. <code>glocal</code> is the output vector. <code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> .
Return value	A <code>CVLocalFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODE</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CVode</code> returns <code>CV_LSETUP_FAIL</code>).
Notes	This function must assume that all interprocess communication of data needed to calculate <code>glocal</code> has already been done, and that this data is accessible within <code>user_data</code> . The case where g is mathematically identical to f is allowed.

CVCommFn

Definition	<code>typedef int (*CVCommFn)(sunindextype Nlocal, realtype t, N_Vector y, void *user_data);</code>
Purpose	This <code>cfm</code> function performs all interprocess communication necessary for the execution of the <code>gloc</code> function above, using the input vector <code>y</code> .
Arguments	<code>Nlocal</code> is the local vector length. <code>t</code> is the value of the independent variable. <code>y</code> is the dependent variable. <code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> .
Return value	A <code>CVCommFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODE</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CVode</code> returns <code>CV_LSETUP_FAIL</code>).
Notes	The <code>cfm</code> function is expected to save communicated data in space defined within the data structure <code>user_data</code> . Each call to the <code>cfm</code> function is preceded by a call to the right-hand side function <code>f</code> with the same <code>(t, y)</code> arguments. Thus, <code>cfm</code> can omit any communication done by <code>f</code>

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 `cvode_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 CVODE object
5. Initialize CVODE 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
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 CVODE 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` (`realttype`) 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 CVODE 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 CVODE 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` (`realttype`) 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 CVODE memory block.

`lenrwBBDP` (`long int`) local number of `realttype` 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`

CVBBDPGetNumGfnEvals

Call `flag = CVBBDPGetNumGfnEvals(cvode_mem, &ngevalsBBDP);`

Description The function `CVBBDPGetNumGfnEvals` 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 CVODE 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 `FCVBBDPGetNumGfnEvals`

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 CVODE output and `npsolves` and `nfevalsLS` are linear solver optional outputs (see §4.5.9).

Chapter 5

Using CVODE for Fortran Applications

A Fortran 2003 module (`fcvode_mod`) as well as a Fortran 77 style interface (`FCVODE`) are provided to support the use of `CVODE`, for the solution of ODE systems $dy/dt = f(t, y)$, in a mixed Fortran/C setting. While `CVODE` is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in Fortran.

5.1 CVODE Fortran 2003 Interface Module

The `fcvode_mod` Fortran module defines interfaces to most `CVODE` 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 `CVODE` function `CVodeCreate` is interfaced as `FCVodeCreate`. Thus, the steps to use `CVODE` and the function calls in Fortran 2003 are identical (ignoring language differences) to those in C. The C functions with Fortran 2003 interfaces indicate this in their description in Chapter 4. The Fortran 2003 `CVODE` interface module can be accessed by the `use` statement, i.e. `use fcvode_mod`, and linking to the library `libsundials_fcvode_mod.lib` in addition to `libsundials_cvode.lib`.

The Fortran 2003 interface modules were generated with SWIG Fortran, a fork of SWIG [34]. Users who are interested in the SWIG code used in the generation process should contact the SUNDIALS development team.

5.1.1 SUNDIALS Fortran 2003 Interface Modules

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

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

Further information on the Fortran 2003 interfaces specific to modules is given in the `NVECTOR`, `SUNMATRIX`, `SUNLINSOL`, and `SUNNONLINSOL` alongside the C documentation (chapters 6, 7, 8, and 9

respectively). For details on where the Fortran 2003 module (.mod) files and libraries are installed see Appendix A.

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

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

5.1.2 Data Types

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



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

Table 5.2: C/Fortran 2003 Equivalent Types

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

5.1.3 Notable Fortran/C usage differences

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

5.1.3.1 Creating generic SUNDIALS objects

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

C code:

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

Fortran code:

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

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

5.1.3.2 Arrays and pointers

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

C code:

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

x = N_VNew_Serial(N);

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

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

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

Fortran code:

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

x => FN_VNew_Serial(x)

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

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

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

5.1.3.3 Passing procedure pointers and user data

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

Typically when passing user data to a SUNDIALS function, a user may simply cast some custom data structure as a `void*`. When using the Fortran 2003 interfaces, the same thing can be achieved.

Note, the custom data structure *does not* have to be `bind(C)` since it is never accessed on the C side.

C code:

```
MyUserData* udata;
void *cvoice_mem;

ierr = CvoiceSetUserData(cvoice_mem, udata);
```

Fortran code:

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

ierr = FCvoiceSetUserData(cvoice_mem, c_loc(udata))
```

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

5.1.3.4 Passing NULL to optional parameters

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

C code:

```
SUNLinearSolver LS;
N_Vector x, b;

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

Fortran code:

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

A => null()

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

5.1.3.5 Working with N_Vector arrays

Arrays of `N_Vector` objects are interfaced to Fortran 2003 as opaque `type(c_ptr)`. As such, it is not possible to directly index an array of `N_Vector` objects returned by the `N_Vector` “VectorArray” operations, or packages with sensitivity capabilities. 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 6.1.5.

5.1.3.6 Providing file pointers

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

FSUNDIALSFileOpen

Call `fp = FSUNDIALSFileOpen(filename, mode)`

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

Arguments `filename` (`character(kind=C_CHAR, len=*)`) - the path to the file to open
`mode` (`character(kind=C_CHAR, len=*)`) - the mode string given to `fopen`. It should begin with one of the following characters:

“r” - open text file for reading

“r+” - open text file for reading and writing

“w” - truncate text file to zero length or create it for writing

“w+” - open text file for reading or writing, create it if it does not exist

“a” - open for appending, see documentation of “fopen” for your system/compiler

“a+” - open for reading and appending, see documentation for “fopen” for your system/compiler

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

FSUNDIALSFileClose

Call `call FSUNDIALSFileClose(fp)`

Description The function deallocates a `FILE*` by calling the C function `fclose`.

Arguments `fp` (`type(C_PTR)`) - the file pointer (type `FILE*` in C)

Return value None

5.1.4 Important notes on portability

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

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

5.2 FCVODE, an Interface Module for FORTRAN Applications

The FCVODE interface module is a package of C functions which support the use of the CVODE. This package provides the necessary interface to CVODE for all supplied serial and parallel NVECTOR implementations.

5.2.1 Important note on portability

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

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

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

5.2.2 Fortran Data Types

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

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

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

- `int64_t` – equivalent to an `INTEGER*8` in FORTRAN

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

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

- `single` – equivalent to a `REAL` or `REAL*4` in FORTRAN
- `double` – equivalent to a `DOUBLE PRECISION` or `REAL*8` in FORTRAN
- `extended` – equivalent to a `REAL*16` in FORTRAN

5.2.3 FCVODE routines

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

- Interface to the NVECTOR modules
 - `FNVINITS` (defined by `NVECTOR_SERIAL`) interfaces to `N_VNewEmpty_Serial`.
 - `FNVINITP` (defined by `NVECTOR_PARALLEL`) interfaces to `N_VNewEmpty_Parallel`.
 - `FNVINITOMP` (defined by `NVECTOR_OPENMP`) interfaces to `N_VNewEmpty_OpenMP`.
 - `FNVINITPTS` (defined by `NVECTOR_PTHREADS`) interfaces to `N_VNewEmpty_Pthreads`.
- Interface to the SUNMATRIX modules
 - `FSUNBANDMATINIT` (defined by `SUNMATRIX_BAND`) interfaces to `SUNBandMatrix`.
 - `FSUNDENSEMATINIT` (defined by `SUNMATRIX_DENSE`) interfaces to `SUNDenseMatrix`.
 - `FSUNSPARSEMATINIT` (defined by `SUNMATRIX_SPARSE`) interfaces to `SUNSparseMatrix`.
- Interface to the SUNLINSOL modules
 - `FSUNBANDLINSOLINIT` (defined by `SUNLINSOL_BAND`) interfaces to `SUNLinSol_Band`.
 - `FSUNDENSELINSOLINIT` (defined by `SUNLINSOL_DENSE`) interfaces to `SUNLinSol_Dense`.
 - `FSUNKLUINIT` (defined by `SUNLINSOL_KLU`) interfaces to `SUNLinSol_KLU`.
 - `FSUNKLUREINIT` (defined by `SUNLINSOL_KLU`) interfaces to `SUNLinSol_KLUReminit`.
 - `FSUNLAPACKBANDINIT` (defined by `SUNLINSOL_LAPACKBAND`) interfaces to `SUNLinSol_LapackBand`.
 - `FSUNLAPACKDENSEINIT` (defined by `SUNLINSOL_LAPACKDENSE`) interfaces to `SUNLinSol_LapackDense`.
 - `FSUNPCGINIT` (defined by `SUNLINSOL_PCG`) interfaces to `SUNLinSol_PCG`.
 - `FSUNSPBCGSINIT` (defined by `SUNLINSOL_SPBCGS`) interfaces to `SUNLinSol_SPBCGS`.
 - `FSUNSPFGMRINIT` (defined by `SUNLINSOL_SPFGMR`) interfaces to `SUNLinSol_SPFGMR`.
 - `FSUNSPGMRINIT` (defined by `SUNLINSOL_SPGMR`) interfaces to `SUNLinSol_SPGMR`.
 - `FSUNSPTFQMRINIT` (defined by `SUNLINSOL_SPTFQMR`) interfaces to `SUNLinSol_SPTFQMR`.
 - `FSUNSUPERLUMTINIT` (defined by `SUNLINSOL_SUPERLUMT`) interfaces to `SUNLinSol_SuperLUMT`.
- Interface to the main CVODE module
 - `FCVMALLOC` interfaces to `CVodeCreate`, `CVodeSetUserData`, and `CVodeInit`, as well as one of `CVodeSStolerances` or `CVodeSVtolerances`.

- FCVREINIT interfaces to C`VodeReInit`.
 - FCVSETIIN and FCVSETRIN interface to C`VodeSet*` functions.
 - FCVWEIGHTSET interfaces to C`VodeWFtolerances`.
 - FCVODE interfaces to C`Vode`, C`VodeGet*` functions, and to the optional output functions for the selected linear solver module.
 - FCVDKY interfaces to the interpolated output function C`VodeGetDky`.
 - FCVGETERRWEIGHTS interfaces to C`VodeGetErrWeights`.
 - FCVGETESTLOCALERR interfaces to C`VodeGetEstLocalErrors`.
 - FCVFREE interfaces to C`VodeFree`.
- Interface to the linear solver interfaces
 - FCVLSINIT interfaces to C`VodeSetLinearSolver`.
 - FCVLSSETEPSLIN interfaces to C`VodeSetEpsLin`.
 - FCVLSSETJAC interfaces to C`VodeSetJacTimes`.
 - FCVLSSETPREC interfaces to C`VodeSetPreconditioner`.
 - FCVDENSESETJAC interfaces to C`VodeSetJacFn`.
 - FCVBANDSETJAC interfaces to C`VodeSetJacFn`.
 - FCVSPARSESETJAC interfaces to C`VodeSetJacFn`.
 - FCVDIAG interfaces to C`VDiag`.
 - Interface to the nonlinear solver interface
 - FCVNLSINIT interfaces to C`VSetNonlinearSolver`.

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

FCVODE routine (FORTRAN, user-supplied)	CVODE function (C, interface)	CVODE type of interface function
FCVFUN	FCVf	CVRhsFn
FCVEWT	FCVEwtSet	CVEwtFn
FCVDJAC	FCVDenseJac	CVLsJacFn
FCVBJAC	FCVBandJac	CVLsJacFn
FCVSPJAC	FCVSparsJac	CVLsJacFn
FCVPSOL	FCVPSol	CVLsPrecSolveFn
FCVPSET	FCVPSet	CVLsPrecSetupFn
FCVJTICES	FCVJtimes	CVLsJacTimesVecFn
FCVJTSETUP	FCVJTSetup	CVLsJacTimesSetupFn

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

5.2.4 Usage of the FCVODE interface module

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

1. Right-hand side specification

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

```
SUBROUTINE FCVFUN(T, Y, YDOT, IPAR, RPAR, IER)
  DIMENSION Y(*), YDOT(*), IPAR(*), RPAR(*)
```

It must set the YDOT array to $f(t, y)$, the right-hand side of the ODE system, as function of $T = t$ and the array $Y = y$. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted).

2. NVECTOR module initialization

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

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

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

3. SUNMATRIX module initialization

If using a nonlinear solver that requires a linear solver (e.g., the default Newton iteration) and the linear solver is a direct linear solver, then one of the SUNMATRIX modules supplied with SUNDIALS, the user must make a call of the form

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

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

4. SUNLINSOL module initialization

If using a nonlinear solver that requires a linear solver (e.g., the default Newton iteration) and one of the SUNLINSOL linear solver modules supplied with SUNDIALS, the user must make a call of the form

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

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

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

```

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

```

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

5. SUNNONLINSOL module initialization

By default CVODE uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL_NEWTON module (see §9.3). To specify a non-default nonlinear solver in CVODE, the user's program must create a SUNNONLINSOL object by calling the appropriate FORTRAN interface function to the constructor routine (see Chapter 9). For example, to create the SUNNONLINSOL_FIXEDPOINT solver call the function

```
CALL FSUNFIXEDPOINTINIT(...)
```

in which the call sequence is described in §9.4.

6. Problem specification

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

FCVMALLOC

Call	CALL FCVMALLOC(TO, YO, METH, IATOL, RTOL, ATOL, & IOUT, ROUT, IPAR, RPAR, IER)
Description	This function provides required problem and solution specifications, specifies optional inputs, allocates internal memory, and initializes CVODE.
Arguments	<p>TO is the initial value of t.</p> <p>YO is an array of initial conditions.</p> <p>METH specifies the basic integration method: 1 for Adams (nonstiff) or 2 for BDF (stiff).</p> <p>IATOL specifies the type for absolute tolerance ATOL: 1 for scalar or 2 for array. If IATOL= 3, the arguments RTOL and ATOL are ignored and the user is expected to subsequently call FCVEWTSET and provide the function FCVEWT.</p> <p>RTOL is the relative tolerance (scalar).</p> <p>ATOL is the absolute tolerance (scalar or array).</p> <p>IOUT is an integer array of length 21 for integer optional outputs.</p> <p>ROUT is a real array of length 6 for real optional outputs.</p> <p>IPAR is an integer array of user data which will be passed unmodified to all user-provided routines.</p> <p>RPAR is a real array of user data which will be passed unmodified to all user-provided routines.</p>
Return value	IER is a return completion flag. Values are 0 for successful return and -1 otherwise. See printed message for details in case of failure.

Notes The user integer data arrays `IOUT` and `IPAR` must be declared as `INTEGER*4` or `INTEGER*8` according to the C type `long int`.
 Modifications to the user data arrays `IPAR` and `RPAR` inside a user-provided routine will be propagated to all subsequent calls to such routines.
 The optional outputs associated with the main CVODE integrator are listed in Table 5.4.

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

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

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

If the `FCVEWT` routine is provided, then, following the call to `FCVMALLOC`, the user must make the call:

```
CALL FCVEWTSET (FLAG, IER)
```

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

7. Set optional inputs

Call `FCVINSETIIN` and/or `FCVINSETRIN` to set desired optional inputs, if any. See §5.2.5 for details.

8. Linear solver interface specification

To attach the linear solver (and optionally the matrix) objects initialized in steps 3 and 4 above, the user of CVODE must initialize the CVLS linear solver interface. To attach any `SUNLINSOL` object (and optional `SUNMATRIX` object) to CVODE, then following calls to initialize the `SUNLINSOL` (and `SUNMATRIX`) object(s) in steps 3 and 4 above, the user must make the call:

```
CALL FCVLSINIT (IER)
```

`IER` is an error return flag set on 0 on success, `-1` if a memory failure occurred, or `-2` for an illegal input.

The previous routines `FCVDSINIT` and `FCVSPILSINIT` 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.

CVLS with dense Jacobian matrix

As an option when using the CVLS interface with the `SUNLINSOL_DENSE` or `SUNLINSOL_LAPACKDENSE` linear solvers, the user may supply a routine that computes a dense approximation of the system Jacobian $J = \partial f / \partial y$. If supplied, it must have the following form:

```
SUBROUTINE FCVDJAC (NEQ, T, Y, FY, DJAC, H, IPAR, RPAR,
&                  WK1, WK2, WK3, IER)
  DIMENSION Y(*), FY(*), DJAC(NEQ,*), IPAR(*), RPAR(*),
&                  WK1(*), WK2(*), WK3(*)
```

Typically this routine will use only NEQ, T, Y, and DJAC. It must compute the Jacobian and store it columnwise in DJAC. The input arguments T, Y, and FY contain the current values of t , y , and $f(t, y)$, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC. The vectors WK1, WK2, and WK3 of length NEQ are provided as work space for use in FCVDJAC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if FCVDJAC failed unrecoverably (in which case the integration is halted). NOTE: The argument NEQ has a type consistent with C type `long int` even in the case when the LAPACK dense solver is to be used.

If the user's FCVDJAC uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. The array EWT can be obtained by calling FCVGETERRWEIGHTS using one of the work arrays as temporary storage for EWT. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using either RPAR or a common block.

If the FCVDJAC routine is provided, then, following the call to FCVLSINIT, the user must make the call:

```
CALL FCVDENSESETJAC (FLAG, IER)
```

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

CVLS with band Jacobian matrix

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

```
SUBROUTINE FCVBJAC(NEQ, MU, ML, MDIM, T, Y, FY, BJAC, H, IPAR, RPAR,
&                  WK1, WK2, WK3, IER)
  DIMENSION Y(*), FY(*), BJAC(MDIM,*), IPAR(*), RPAR(*),
&                  WK1(*), WK2(*), WK3(*)
```

Typically this routine will use only NEQ, MU, ML, T, Y, and BJAC. It must load the MDIM by N array BJAC with the Jacobian matrix at the current (t, y) in band form. Store in $BJAC(k, j)$ the Jacobian element $J_{i,j}$ with $k = i - j + MU + 1$ ($k = 1 \cdots ML + MU + 1$) and $j = 1 \cdots N$. The input arguments T, Y, and FY contain the current values of t , y , and $f(t, y)$, respectively. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC. The vectors WK1, WK2, and WK3 of length NEQ are provided as work space for use in FCVBJAC. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if FCVBJAC failed unrecoverably (in which case the integration is halted). NOTE: The arguments NEQ, MU, ML, and MDIM have a type consistent with C type `long int` even in the case when the LAPACK band solver is to be used.

If the user's FCVBJAC uses difference quotient approximations, it may need to use the error weight array EWT and current stepsize H in the calculation of suitable increments. The array EWT can be obtained by calling FCVGETERRWEIGHTS using one of the work arrays as temporary storage for EWT. It may also need the unit roundoff, which can be obtained as the optional output ROUT(6), passed from the calling program to this routine using either RPAR or a common block.

If the FCVBJAC routine is provided, then, following the call to FCVLSINIT, the user must make the call:

```
CALL FCVBANDSETJAC(FLAG, IER)
```

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

CVLS with sparse Jacobian matrix

When using the CVLS interface with the `SUNLINSOL_KLU` or `SUNLINSOL_SUPERLUMT` linear solvers, the user must supply the `FCVSPJAC` routine that computes a compressed-sparse-column or compressed-sparse-row approximation of the system Jacobian $J = \partial f / \partial y$. If supplied, it must have the following form:

```
SUBROUTINE FCVSPJAC(T, Y, FY, N, NNZ, JDATA, JINDEXVALS,
&                  JINDEXPTRS, H, IPAR, RPAR, WK1, WK2, WK3, IER)
```

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

To indicate that the `FCVSPJAC` routine has been provided, then following the call to `FCVLSINIT`, the following call must be made

```
CALL FCVSPARSESETJAC (IER)
```

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

CVLS with Jacobian-vector product

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

```
SUBROUTINE FCVJTIMES (V, FJV, T, Y, FY, H, IPAR, RPAR, WORK, IER)
DIMENSION V(*), FJV(*), Y(*), FY(*), IPAR(*), RPAR(*), WORK(*)
```

Typically this routine will use only `T`, `Y`, `V`, and `FJV`. It must compute the product vector Jv , where the vector v is stored in `V`, and store the product in `FJV`. The input arguments `T`, `Y`, and `FY` contain the current values of t , y , and $f(t, y)$, respectively. On return, set `IER` = 0 if `FCVJTIMES` was successful, and nonzero otherwise. The arrays `IPAR` (of integers) and `RPAR` (of reals) contain user data and are the same as those passed to `FCVMALLOC`. The vector `WORK`, of length commensurate with the input `Y0` to `FCVMALLOC`, is provided as work space for use in `FCVJTIMES`.

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

```
SUBROUTINE FCVJTSETUP (T, Y, FY, H, IPAR, RPAR, IER)
DIMENSION Y(*), FY(*), IPAR(*), RPAR(*)
```

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

To indicate that the FCVJTIMES and FCVJTSETUP routines have been provided, then following the call to FCVLSINIT, the following call must be made

```
CALL FCVLSSETJAC (FLAG, IER)
```

with FLAG $\neq 0$ to specify use of the user-supplied Jacobian-times-vector setup and product routines. The argument IER is an error return flag which is 0 for success or non-zero if an error occurred.

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

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



Notes

- (a) If the user's FCVJTIMES routine uses difference quotient approximations, it may need to use the error weight array EWT, the current stepsize H, and/or the unit roundoff, in the calculation of suitable increments.
- (b) If needed in FCVJTIMES or FCVJTSETUP, the error weight array EWT can be obtained by calling FCVGETERRWEIGHTS using a user-allocated array as temporary storage for EWT.
- (c) If needed in FCVJTIMES or FCVJTSETUP, the unit roundoff can be obtained as the optional output ROUT(6) (available after the call to FCVMALLOC) and can be passed using either the RPAR user data array, a common block or a module.

CVLS with preconditioning

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

```
SUBROUTINE FCVPSOL(T, Y, FY, R, Z, GAMMA, DELTA, LR, IPAR, RPAR, IER)
DIMENSION Y(*), FY(*), R(*), Z(*), IPAR(*), RPAR(*)
```

It must solve the preconditioner linear system $Pz = r$, where $r = R$ is input, and store the solution z in Z. Here P is the left preconditioner if LR=1 and the right preconditioner if LR=2. The preconditioner (or the product of the left and right preconditioners if both are nontrivial) should be an approximation to the matrix $I - \gamma J$, where I is the identity matrix, J is the system Jacobian, and $\gamma = \text{GAMMA}$. The input arguments T, Y, and FY contain the current values of t , y , and $f(t, y)$, respectively. On return, set IER = 0 if FCVPSOL was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred.

The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC.

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

```
SUBROUTINE FCVPSET(T, Y, FY, JOK, JCUR, GAMMA, H, IPAR, RPAR, IER)
DIMENSION Y(*), FY(*), EWT(*), IPAR(*), RPAR(*)
```

It must perform any evaluation of Jacobian-related data and preprocessing needed for the solution of the preconditioner linear systems by FCVPSOL. The input argument JOK allows for Jacobian data to be saved and reused: If JOK = 0, this data should be recomputed from scratch. If JOK = 1, a saved copy of it may be reused, and the preconditioner constructed from it. The input arguments T, Y, and FY contain the current values of t , y , and $f(t, y)$, respectively. On return, set JCUR = 1 if Jacobian data was computed, and set JCUR = 0 otherwise. Also on return, set IER = 0 if FCVPSET was successful, set IER positive if a recoverable error occurred, and set IER negative if a non-recoverable error occurred.

The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC.

To indicate that the FCVPSET and FCVPSOL routines are supplied, then the user must call

```
CALL FCVLSSETPREC(FLAG, IER)
```

with FLAG \neq 0. The return flag IER is 0 if successful, or negative if a memory error occurred. In addition, the user program must include preconditioner routines FCVPSOL and FCVPSET.

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



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

Notes

- (a) If the user's FCVPSET routine uses difference quotient approximations, it may need to use the error weight array EWT, the current stepsize H, and/or the unit roundoff, in the calculation of suitable increments. Also, if FCVPSOL uses an iterative method in its solution, the residual vector $\rho = r - Pz$ of the system should be made less than DELTA in weighted ℓ_2 norm, i.e. $\sqrt{\sum(\rho_i * EWT[i])^2} < DELTA$.
- (b) If needed in FCVPSOL or FCVPSET, the error weight array EWT can be obtained by calling FCVGETERRWEIGHTS using a user-allocated array as temporary storage for EWT.
- (c) If needed in FCVPSOL or FCVPSET, the unit roundoff can be obtained as the optional output ROUT(6) (available after the call to FCVMALLOC) and can be passed using either the RPAR user data array, a common block or a module.

CVDIAG diagonal linear solver interface

CVODE is also packaged with a CVODE-specific diagonal approximate Jacobian and linear solver interface. This choice is appropriate when the Jacobian can be well-approximated by a diagonal matrix. The user must make the call:

```
CALL FCVDIAG(IER)
```

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

There are no additional user-supplied routines for the CVDIAG interface.

Optional outputs specific to the CVDIAG case are listed in Table 5.4.

9. Nonlinear solver interface specification

If a non-default SUNNONLINSOL object was created in step 5, the user must attach it to CVODE with the call:

```
CALL FCVNLSINIT(IER)
```

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

Once attached, the user may specify non-default inputs for the SUNNONLINSOL object (e.g. the maximum number of nonlinear iterations) by calling appropriate FORTRAN interface routines (see Chapter 9).

10. Problem solution

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

```
CALL FCVODE(TOUT, T, Y, ITASK, IER)
```

The arguments are as follows. TOUT specifies the next value of t at which a solution is desired (input). T is the value of t reached by the solver on output. Y is an array containing the computed solution on output. ITASK is a task indicator and should be set to 1 for normal mode (overshoot TOUT and interpolate), or to 2 for one-step mode (return after each internal step taken). IER is a completion flag and will be set to a positive value upon successful return or to a negative value if an error occurred. These values correspond to the CVode returns (see §4.5.6 and §B.2). The current values of the optional outputs are available in IOUT and ROUT (see Table 5.4).

11. Additional solution output

After a successful return from FCVODE, the routine FCVDKY may be used to obtain a derivative of the solution, of order up to the current method order, at any t within the last step taken. For this, make the following call:

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

where T is the value of t at which solution derivative is desired, and K is the derivative order ($0 \leq K \leq QU$). On return, DKY is an array containing the computed K-th derivative of y . The value T must lie between TCUR - HU and TCUR. The return flag IER is set to 0 upon successful return or to a negative value to indicate an illegal input.

12. Problem reinitialization

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

```
CALL FCVREINIT(TO, YO, IATOL, RTOL, ATOL, IER)
```

The arguments have the same names and meanings as those of FCMALLOC. FCVREINIT performs the same initializations as FCMALLOC, but does no memory allocation, using instead the existing internal memory created by the previous FCMALLOC call. The call to specify the linear system solution method may or may not be needed.

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

13. Memory deallocation

To free the internal memory created by the call to FCMALLOC, FCVLSINIT, FNVINIT* and FSUN***MATINIT, make the call

```
CALL FCVFREE
```

Table 5.3: Keys for setting FCVODE optional inputs

Integer optional inputs (FCVSETIIN)		
Key	Optional input	Default value
MAX_ORD	Maximum LMM method order	5 (BDF), 12 (Adams)
MAX_NSTEPS	Maximum no. of internal steps before t_{out}	500
MAX_ERRFAIL	Maximum no. of error test failures	7
MAX_NITERS	Maximum no. of nonlinear iterations	3
MAX_CONVFAIL	Maximum no. of convergence failures	10
HNIL_WARNMS	Maximum no. of warnings for $t_n + h = t_n$	10
STAB_LIM	Flag to activate stability limit detection	0

Real optional inputs (FCVSETRIN)		
Key	Optional input	Default value
INIT_STEP	Initial step size	estimated
MAX_STEP	Maximum absolute step size	∞
MIN_STEP	Minimum absolute step size	0.0
STOP_TIME	Value of t_{stop}	undefined
NLCONV_COEF	Coefficient in the nonlinear convergence test	0.1

Real vector optional inputs (FCVSETVIN)		
Key	Optional Input	Default value
CONSTR_VEC	Inequality constraints on solution	undefined

5.2.5 FCVODE optional input and output

In order to keep the number of user-callable FCVODE interface routines to a minimum, optional inputs to the CVODE solver are passed through only three routines: FCVSETIIN for integer optional inputs, FCVSETRIN for real optional inputs, and FCVSETVIN for real vector (array) optional inputs. These functions should be called as follows:

```
CALL FCVSETIIN(KEY, IVAL, IER)
CALL FCVSETRIN(KEY, RVAL, IER)
CALL FCVSETVIN(KEY, VVAL, IER)
```

where KEY is a quoted string indicating which optional input is set (see Table 5.3), IVAL is the integer input value to be used, RVAL is the real input value to be used, VVAL is the real input array to be used, and IER is an integer return flag which is set to 0 on success and a negative value if a failure occurred. The integer IVAL should be declared in a manner consistent with C type `long int`.

When using FCVSETVIN to specify optional constraints on the solution vector (KEY = 'CONSTR_VEC') the components in the array VVAL should be one of -2.0, -1.0, 0.0, 1.0, or 2.0. See the description of CCodeSetConstraints (§4.5.7.1) for details.

The optional outputs from the CVODE solver are accessed not through individual functions, but rather through a pair of arrays, IOUT (integer type) of dimension at least 21, and ROUT (real type) of dimension at least 6. These arrays are owned (and allocated) by the user and are passed as arguments to FCVMALLOC. Table 5.4 lists the entries in these two arrays and specifies the optional variable as well as the CVODE function which is actually called to extract the optional output.

For more details on the optional inputs and outputs, see §4.5.7 and §4.5.9.

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

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

```
CALL FCVGETERRWEIGHTS (EWT, IER)
```

Table 5.4: Description of the FCVODE optional output arrays IOUT and ROUT

Integer output array IOUT		
Index	Optional output	CVODE function
CVODE main solver		
1	LENRW	CVodeGetWorkSpace
2	LENIW	CVodeGetWorkSpace
3	NST	CVodeGetNumSteps
4	NFE	CVodeGetNumRhsEvals
5	NETF	CVodeGetNumErrTestFails
6	NCFN	CVodeGetNumNonlinSolvConvFails
7	NNI	CVodeGetNumNonlinSolvIters
8	NSETUPS	CVodeGetNumLinSolvSetups
9	QU	CVodeGetLastOrder
10	QCUR	CVodeGetCurrentOrder
11	NOR	CVodeGetNumStabLimOrderReds
12	NGE	CVodeGetNumGEvals
CVLS linear solver interface		
13	LENRWLS	CVodeGetLinWorkSpace
14	LENIWLS	CVodeGetLinWorkSpace
15	LS_FLAG	CVodeGetLastLinFlag
16	NFELS	CVodeGetNumLinRhsEvals
17	NJE	CVodeGetNumJacEvals
18	NJTS	CVodeGetNumJTSetupEvals
19	NJTV	CVodeGetNumJtimesEvals
20	NPE	CVodeGetNumPrecEvals
21	NPS	CVodeGetNumPrecSolves
22	NLI	CVodeGetNumLinIters
23	NCFL	CVodeGetNumLinConvFails
CVDIAG linear solver interface		
13	LENRWLS	CVdiagGetWorkSpace
14	LENIWLS	CVdiagGetWorkSpace
15	LS_FLAG	CVdiagGetLastFlag
16	NFELS	CVdiagGetNumRhsEvals

Real output array ROUT		
Index	Optional output	CVODE function
1	HOU	CVodeGetActualInitStep
2	HU	CVodeGetLastStep
3	HCUR	CVodeGetCurrentStep
4	TCUR	CVodeGetCurrentTime
5	TOLSF	CVodeGetTolScaleFactor
6	UROUND	unit roundoff

This computes the EWT array normally defined by Eq. (2.7). The array EWT, of length NEQ or NLOCAL, must already have been declared by the user. The error return flag IER is zero if successful, and negative if there was a memory error.

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

```
CALL FCVGETESTLOCALERR (ELE, IER)
```

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

5.2.6 Usage of the FCVROOT interface to rootfinding

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

- FCVROOTINIT interfaces to CCodeRootInit.
- FCVROOTINFO interfaces to CCodeGetRootInfo.
- FCVROOTFREE interfaces to CCodeRootFree.

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

In order to use the rootfinding feature of CVODE, the following call must be made, after calling FCVMALLOC but prior to calling FCVODE, to allocate and initialize memory for the FCVROOT module:

```
CALL FCVROOTINIT (NRTFN, IER)
```

The arguments are as follows: NRTFN is the number of root functions. IER is a return completion flag; its values are 0 for success, -1 if the CVODE memory was NULL, and -11 if a memory allocation failed.

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

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

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

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

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

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

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

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

```
CALL FCVROOTFREE
```

5.2.7 Usage of the FCVBP interface to CVBANDPRE

The FCVBP interface sub-module is a package of C functions which, as part of the FCVODE interface module, support the use of the CVOICE solver with the serial NVECTOR_SERIAL module or multi-threaded NVECTOR_OPENMP or NVECTOR_PTHREADS, and the combination of the CVBANDPRE preconditioner module (see §4.7.1) with the CVLS interface and any of the Krylov iterative linear solvers.

The two user-callable functions in this package, with the corresponding CVOICE function around which they wrap, are:

- FCVBPINIT interfaces to CVBandPrecInit.
- FCVBP OPT interfaces to CVBANDPRE optional output functions.

As with the rest of the FCVODE routines, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fcvbp.h`.

The following is a summary of the usage of this module. Steps that are unchanged from the main program described in §5.2.4 are grayed-out.

1. Right-hand side specification

2. NVECTOR module initialization

3. SUNLINSOL module initialization

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

4. SUNNONLINSOL module initialization

5. Problem specification

6. Set optional inputs

7. Linear solver interface specification

First, initialize the CVLS linear solver interface by calling FCVLSINIT.

Then, to initialize the CVBANDPRE preconditioner, make the following call:

```
CALL FCVBPINIT(NEQ, MU, ML, IER)
```

The arguments are as follows. NEQ is the problem size. MU and ML are the upper and lower half-bandwidths of the band matrix that is retained as an approximation of the Jacobian. IER is a return completion flag. A value of 0 indicates success, while a value of -1 indicates that a memory failure occurred.

Optionally, to specify that CVLS should use the supplied FCVJTIMES and FCVJTSETUP, make the call

```
CALL FCVLSSETJAC(FLAG, IER)
```

with FLAG \neq 0 (see step 8 in §5.2.4 for details).

8. Nonlinear solver interface specification

9. Problem solution

10. Additional solution output

11. CVBANDPRE Optional outputs

Optional outputs specific to the CVLS solver interface are listed in Table 5.4. To obtain the optional outputs associated with the CVBANDPRE module, make the following call:

```
CALL FCVBPOPT(LENRWBP, LENIWBP, NFEBP)
```

The arguments should be consistent with C type `long int`. Their returned values are as follows: `LENRWBP` is the length of real preconditioner work space, in `realtype` words. `LENIWBP` is the length of integer preconditioner work space, in integer words. `NFEBP` is the number of $f(t, y)$ evaluations (calls to `FCVFUN`) for difference-quotient banded Jacobian approximations.

12. Memory deallocation

(The memory allocated for the `FCVBP` module is deallocated automatically by `FCVFREE`.)

5.2.8 Usage of the FCVBBD interface to CVBBDPRE

The `FCVBBD` interface sub-module is a package of C functions which, as part of the `FCVODE` interface module, support the use of the `CVODE` solver with the parallel `NVECTOR_PARALLEL` module, and the combination of the `CVBBDPRE` preconditioner module (see §4.7.2) with any of the Krylov iterative linear solvers.

The user-callable functions in this package, with the corresponding `CVODE` and `CVBBDPRE` functions, are as follows:

- `FCVBBDINIT` interfaces to `CVBBDPrecInit`.
- `FCVBBDREINIT` interfaces to `CVBBDPrecReInit`.
- `FCVBBDOPT` interfaces to `CVBBDPRE` optional output functions.

In addition to the FORTRAN right-hand side function `FCVFUN`, the user-supplied functions used by this package, are listed below, each with the corresponding interface function which calls it (and its type within `CVBBDPRE` or `CVODE`):

FCVBBD routine (FORTRAN, user-supplied)	CVODE function (C, interface)	CVODE type of interface function
<code>FCVLOCFN</code>	<code>FCVgloc</code>	<code>CVLocalFn</code>
<code>FCVCOMMF</code>	<code>FCVcfn</code>	<code>CVCommFn</code>
<code>FCVJTIMES</code>	<code>FCVJtimes</code>	<code>CVLsJacTimesVecFn</code>
<code>FCVJTSETUP</code>	<code>FCVJTSetup</code>	<code>CVLsJacTimesSetupFn</code>

As with the rest of the `FCVODE` routines, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program. Additionally, based on flags discussed above in §5.2.3, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fcvbbd.h`.

The following is a summary of the usage of this module. Steps that are unchanged from the main program described in §5.2.4 are grayed-out.

1. **Right-hand side specification**
2. `NVECTOR` module initialization
3. `SUNLINSOL` module initialization

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

4. `SUNNONLINSOL` module initialization
5. **Problem specification**
6. **Set optional inputs**

7. Linear solver interface specification

First, initialize the CVLS iterative linear solver interface by calling FCVLSINIT.

Then, to initialize the CVBBDPRE preconditioner, make the following call:

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

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

Optionally, to specify that SPGMR, SPBCGS, or SPTFQMR should use the supplied FCVJTIMES, make the call

```
CALL FCVLSSETJAC(FLAG, IER)
```

with FLAG $\neq 0$ (see step 8 in §5.2.4 for details).

8. Nonlinear solver interface specification

9. Problem solution

10. Additional solution output

11. CVBBDPRE **Optional outputs**

Optional outputs specific to the CVLS solver interface are listed in Table 5.4. To obtain the optional outputs associated with the CVBBDPRE module, make the following call:

```
CALL FCVBBDOPT(LENRWBBD, LENIWBBBD, NGEBBD)
```

The arguments should be consistent with C type long int. Their returned values are as follows: LENRWBBD is the length of real preconditioner work space, in realtype words. LENIWBBBD is the length of integer preconditioner work space, in integer words. These sizes are local to the current processor. NGEBBD is the number of $g(t, y)$ evaluations (calls to FCVLOCFN) so far.

12. Problem reinitialization

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

```
CALL FCVBBDREINIT(NLOCAL, MUDQ, MLDQ, DQRELY, IER)
```

This reinitializes the CVBBDPRE preconditioner, but without reallocating its memory. The arguments of the FCVBBDREINIT routine have the same names and meanings as those of FCVBBDINIT. If the value of MU or ML is being changed, then a call to FCVBBDINIT must be made. Finally, if there is a change in any of the linear solver inputs, then a call to one of FSUNPCGINIT, FSUNSPBCGSINIT, FSUNSPFGMRINIT, FSUNSPGMRINIT or FSUNSPTFQMRINIT, followed by a call to FCVLSINIT must also be made; in this case the linear solver memory is reallocated.

13. Memory deallocation

(The memory allocated for the FCVBBD module is deallocated automatically by FCVFREE.)

14. User-supplied routines

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

```
SUBROUTINE FCVGLOCFN (NLOC, T, YLOC, GLOC, IPAR, RPAR, IER)
  DIMENSION YLOC(*), GLOC(*), IPAR(*), RPAR(*)
```

This routine is to evaluate the function $g(t, y)$ approximating f (possibly identical to f), in terms of $T = t$, and the array $YLOC$ (of length $NLOC$), which is the sub-vector of y local to this processor. The resulting (local) sub-vector is to be stored in the array $GLOC$. The arrays $IPAR$ (of integers) and $RPAR$ (of reals) contain user data and are the same as those passed to $FCVMALLOC$. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if $FCVGLOCFN$ failed unrecoverably (in which case the integration is halted).

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

This routine is to perform the inter-processor communication necessary for the $FCVGLOCFN$ routine. Each call to $FCVCOMMFN$ is preceded by a call to the right-hand side routine $FCVFUN$ with the same arguments T and $YLOC$. The arrays $IPAR$ (of integers) and $RPAR$ (of reals) contain user data and are the same as those passed to $FCVMALLOC$. IER is an error return flag (currently not used; set $IER=0$). Thus $FCVCOMMFN$ can omit any communications done by $FCVFUN$ if relevant to the evaluation of $GLOC$. IER is an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if $FCVCOMMFN$ failed unrecoverably (in which case the integration is halted).



The subroutine $FCVCOMMFN$ must be supplied even if it is not needed and must return $IER=0$.

Optionally, the user can supply routines $FCVJTIMES$ and $FCVJTSETUP$ for the evaluation of Jacobian-vector products, as described above in step 8 in §5.2.4.

Chapter 6

Description of the NVECTOR module

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

6.1 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.

6.1.1 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 6.1.

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 `realtyp` array from the `N_Vector` `v`. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtyp`. 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 `realtyp*`

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`: $z_i = ax_i + by_i$, $i = 0, \dots, n - 1$.

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 `realtypc` `c`: $z_i = c, i = 0, \dots, n - 1$.

Arguments `c` (`realtypc`) 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`:
 $z_i = x_i y_i, i = 0, \dots, n - 1$.

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`:
 $z_i = x_i / y_i, i = 0, \dots, n - 1$. 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 `realtypc` scalar `c` and returns the result in `z`: $z_i = c x_i, i = 0, \dots, n - 1$.

Arguments `c` (`realtypc`) 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`: $y_i = |x_i|$, $i = 0, \dots, n - 1$.

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`: $z_i = 1.0/x_i$, $i = 0, \dots, n - 1$. 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 `realtyp` scalar `b` to all components of `x` and returns the result in the `N_Vector` `z`: $z_i = x_i + b$, $i = 0, \dots, n - 1$.

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

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 `realtyp`

F2003 Name `FN_VMaxNorm`

N_VWrmsNorm

Call $m = \text{N_VWrmsNorm}(x, w)$

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 $m = \text{N_VWrmsNormMask}(x, w, id)$;

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 $m = \text{N_VMin}(x)$;

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 $m = \text{N_VWL2Norm}(x, w)$;

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 $m = \text{N_VL1Norm}(x)$;

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

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 `numi` by `denomi`. 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`

6.1.2 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:

$$z_i = \sum_{j=0}^{n_v-1} c_j x_{j,i}, \quad i = 0, \dots, n-1,$$

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`
`ier = 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:

$$z_{j,i} = c_j x_i + y_{j,i}, \quad j = 0, \dots, n_v - 1 \quad i = 0, \dots, n - 1,$$

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 `ierr = N_VDotProdMulti(nv, x, Y, d);`

Description This routine computes the dot product of a vector with n_v other vectors:

$$d_j = \sum_{i=0}^{n-1} x_i y_{j,i}, \quad j = 0, \dots, n_v - 1,$$

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)`

6.1.3 NVECTOR vector array functions

`N_VLinearSumVectorArray`

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

Description This routine computes the linear sum of two vector arrays containing n_v vectors of n elements:

$$z_{j,i} = ax_{j,i} + by_{j,i}, \quad i = 0, \dots, n - 1 \quad j = 0, \dots, n_v - 1,$$

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:

$$z_{j,i} = c_j x_{j,i}, \quad i = 0, \dots, n-1 \quad j = 0, \dots, n_v - 1,$$

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:

$$z_{j,i} = c, \quad i = 0, \dots, n-1 \quad j = 0, \dots, n_v - 1,$$

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:

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

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:

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

$H(id_i) = 1$ 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:

$$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0, \dots, n-1 \quad j = 0, \dots, n_v - 1,$$

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:

$$z_{j,i} = \sum_{k=0}^{n_s-1} c_k x_{k,j,i}, \quad i = 0, \dots, n-1 \quad j = 0, \dots, n_v - 1,$$

where c is an array of n_s scalars (type `realtype*`), XX (type `N_Vector**`) is an array of n_s vector arrays each containing n_v vectors to be summed into the output vector array of n_v vectors Z (type `N_Vector*`). If the output vector array Z is one of the vector arrays in XX , then it *must* be the first vector array in XX .

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.

6.1.4 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 6.14). 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`:

$$m = \max_{0 \leq i < n_{local}} |x_i|,$$

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

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

Return value `realtype`

F2003 Name `FN_VMaxNormLocal`

N_VMinLocal

Call `m = N_VMinLocal(x);`

Description This routine computes the smallest element of the MPI task-local portion of the `N_Vector` `x`:

$$m = \min_{0 \leq i < n_{local}} x_i,$$

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

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

Return value `realtype`

F2003 Name `FN_VMinLocal`

`N_VL1NormLocal`

Call `n = N_VL1NormLocal(x);`

Description This routine computes the MPI task-local portion of the ℓ_1 norm of the `N_Vector` `x`:

$$n = \sum_{i=0}^{n_{local}-1} |x_i|,$$

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

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

Return value `realtype`

F2003 Name `FN_VL1NormLocal`

`N_VWSqrSumLocal`

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

Description This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector` `x` with weight vector `w`:

$$s = \sum_{i=0}^{n_{local}-1} (x_i w_i)^2,$$

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

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

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

Return value `realtype`

F2003 Name `FN_VWSqrSumLocal`

`N_VWSqrSumMaskLocal`

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

Description This routine computes the MPI task-local portion of the weighted squared sum of the `N_Vector` `x` with weight vector `w` built using only the elements of `x` corresponding to positive elements of the `N_Vector` `id`:

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

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

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

Return value `realtype`

F2003 Name `FN_VWSqrSumMaskLocal`

`N_VInvTestLocal`

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

Description Sets the MPI task-local components of the `N_Vector` **z** to be the inverses of the components of the `N_Vector` **x**, with prior testing for zero values:

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

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

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:

$$\begin{aligned} x_i > 0 & \quad \text{if } c_i = 2, \\ x_i \geq 0 & \quad \text{if } c_i = 1, \\ x_i \leq 0 & \quad \text{if } c_i = -1, \\ x_i < 0 & \quad \text{if } c_i = -2, \text{ and} \\ \text{no test} & \quad \text{if } c_i = 0, \end{aligned}$$

for all MPI task-local components of the vectors. It sets a mask vector **m**, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.

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

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

F2003 Name `FN_VConstrMaskLocal`

`N_VMinQuotientLocal`

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

Description This routine returns the minimum of the quotients obtained by term-wise dividing num_i by denom_i , for all MPI task-local components of the vectors. A zero element in **denom** will be skipped. If no such quotients are found, then the large value `BIG_REAL` (defined in the header file `sundials_types.h`) is returned.

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

Return value `realtyp`

F2003 Name `FN_VMinQuotientLocal`

6.1.5 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 6.1: Vector Identifications associated with vector kernels supplied with SUNDIALS.

Vector ID	Vector type	ID Value
SUNDIALS_NVEC_SERIAL	Serial	0
SUNDIALS_NVEC_PARALLEL	Distributed memory parallel (MPI)	1
SUNDIALS_NVEC_OPENMP	OpenMP shared memory parallel	2
SUNDIALS_NVEC_PTHREADS	PThreads shared memory parallel	3
SUNDIALS_NVEC_PARHYP	<i>hypre</i> 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`

6.1.6 NVECTOR identifiers

Each NVECTOR implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 6.1.

6.1.7 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 (*nvintest)(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      (*nvlnormlocal)(N_Vector);
boolean_type  (*nvinvtestlocal)(N_Vector, N_Vector);
boolean_type  (*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 6.1.1 defines a complete list of all standard vector operations defined by the generic NVECTOR module. Sections 6.1.2, 6.1.3 and 6.1.4 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 :: nvscaleaddmultivecarray
type(C_FUNPTR), public :: nvlinearcombinationvecarray
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

```

6.1.8 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.

6.1.8.1 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 6.1.1-6.1.4 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., $z_i = c + 0j$, $i = 0, \dots, n - 1$.
- `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`.

6.2 NVECTOR functions used by CVODE

In Table 6.2 below, we list the vector functions in the NVECTOR module used within the `CVODE` package. The table also shows, for each function, which of the code modules uses the function. The `CVODE` column shows function usage within the main integrator module, while the remaining columns show function usage within each of the `CVODE` linear solver interfaces, the `CVBANDPRE` and `CVBBDPRE` preconditioner modules, and the `FCVODE` module. Here `CVLS` stands for the generic linear solver interface in `CVODE`, and `CVDIAG` stands for the diagonal linear solver interface in `CVODE`.

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

Special cases (numbers match markings in table):

Table 6.2: List of vector functions usage by CVOICE code modules

	CVOICE	CVLS	CVDIAG	CVBANDPRE	CVBDDPRE	FCVOICE
N_VGetVectorID						
N_VGetLength		4				
N_VClone	✓	✓	✓			
N_VCloneEmpty		1				✓
N_VDestroy	✓	✓	✓			
N_VSpace	✓	2				
N_VGetArrayPointer		1		✓	✓	✓
N_VSetArrayPointer		1				✓
N_VLinearSum	✓	✓	✓			
N_VConst	✓	✓				
N_VProd	✓		✓			
N_VDiv	✓		✓			
N_VScale	✓	✓	✓	✓	✓	
N_VAbs	✓					
N_VInv	✓		✓			
N_VAddConst	✓		✓			
N_VMaxNorm	✓					
N_VWrmsNorm	✓	✓		✓	✓	
N_VMin	✓					
N_VMinQuotient	✓					
N_VConstrMask	✓					
N_VCompare	✓		✓			
N_VInvTest			✓			
N_VLinearCombination	✓					
N_VScaleAddMulti	✓					
N_VDotProdMulti	3	3				
N_VScaleVectorArray	✓					

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 CVOICE 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`. The remaining operations from Sections 6.1.2 and 6.1.3 not listed above are unused and a user-supplied NVECTOR module for CVOICE could omit these operations.
4. This routine is only used when an iterative or matrix iterative `SUNLINSOL` module is supplied to CVOICE.

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 8.5-8.17 for additional detail on their NVECTOR requirements.

The vector functions listed in Section 6.1.1 that are *not* used by CVOICE are: `N_VWL2Norm`, `N_VDotProd`, `N_VL1Norm`, `N_VWrmsNormMask`, and `N_VGetCommunicator`. Therefore, a user-supplied NVECTOR mod-

ule for CVOICE could omit these functions (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.

6.3 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.

6.3.1 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] )
```

6.3.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3 and 6.1.4. 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 6.1.1 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.



6.3.3 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 `FN_VINITIS(code, NEQ, IER)`, to initialize this `NVECTOR_SERIAL` module. Here `code` is an input solver id (1 for `CVODE`, 2 for `IDA`, 3 for `KINSOL`, 4 for `ARKODE`); `NEQ` is the problem size (declared so as to match C type `long int`); and `IER` is an error return flag equal 0 for success and -1 for failure.

6.4 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.

6.4.1 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] )
```

6.4.2 NVECTOR_PARALLEL functions

The `NVECTOR_PARALLEL` module defines parallel implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. 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, boolean_type 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, boolean_type 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, boolean_type 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, boolean_type 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.



6.4.3 NVECTOR_PARALLEL Fortran interfaces

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



6.5 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`.

6.5.1 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] )
```

6.5.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. 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 6.1.1 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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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.

6.5.3 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 `FNINITOMP(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `NEQ` is the problem size (declared so as to match C type `long int`); `NUMTHREADS` is the number of threads; and `IER` is an error return flag equal 0 for success and -1 for failure.

6.6 The NVECTOR_PTHREADS implementation

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

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

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

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

6.6.1 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] )
```

6.6.2 NVECTOR_PTHREADS functions

The `NVECTOR_PTHREADS` module defines Pthreads implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4. Their names are obtained from those in these tables by appending the suffix `_Pthreads` (e.g. `NV_Destroy_Pthreads`). All the standard vector operations listed in 6.1.1 are callable via the FORTRAN 2003 interface by prepending an ‘F’ (e.g. `FN_NV_Destroy_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.

6.6.3 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 `FNINITPTS(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `NEQ` is the problem size (declared so as to match C type `long int`); `NUMTHREADS` is the number of threads; and `IER` is an error return flag equal 0 for success and -1 for failure.

6.7 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.

6.7.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 [31] and the `ark_diurnal_kry_ph.c` example program for ARKODE [41].

The names of parhyp methods are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 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.

6.8 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.

6.8.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 [30].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 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 recommended to extract the PETSC vector via `x_vec = N_VGetVector_Petsc(v)` and then access components using appropriate PETSC functions.
- The functions `N_VNewEmpty_Petsc`, `N_VMake_Petsc`, and `N_VCloneVectorArrayEmpty_Petsc` set the field `own_data` to `SUNFALSE`. `N_VDestroy_Petsc` and `N_VDestroyVectorArray_Petsc` will not attempt to free the pointer `pvec` for any `N_Vector` with `own_data` set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the `pvec` pointer.
- To maximize efficiency, vector operations in the `NVECTOR_PETSC` implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.



6.9 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.

6.9.1 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 `realtyp *N_VGetHostArrayPointer_Cuda(N_Vector v)`

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

`N_VGetDeviceArrayPointer_Cuda`

Prototype `realtyp *N_VGetDeviceArrayPointer_Cuda(N_Vector v)`

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

`N_VIsManagedMemory_Cuda`

Prototype `booleantyp *N_VIsManagedMemory_Cuda(N_Vector v)`

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

The NVECTOR_CUDA module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3 and 6.1.4, 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 C-ODE [31].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 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(sunindextyp 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 recommended 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.



6.10 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_rajaj.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.

6.10.1 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 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 [31].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4 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 recommended to use functions `N_VGetDeviceArrayPointer_Raja` or `N_VGetHostArrayPointer_Raja`.
- To maximize efficiency, vector operations in the `NVECTOR_RAJA` implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.



6.11 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.

6.11.1 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 )
```

6.11.2 NVECTOR_OPENMPDEV functions

The `NVECTOR_OPENMPDEV` module defines OpenMP device offloading implementations of all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 6.1.1, 6.1.2, 6.1.3, and 6.1.4 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, reatype *h_vdata, reatype *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 `reaotype *N_VGetHostArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the host data array.

N_VGetDeviceArrayPointer_OpenMPDEV

Prototype `reaotype *N_VGetDeviceArrayPointer_OpenMPDEV(N_Vector v)`

Description This function returns a pointer to the device data array.

N_VPrint_OpenMPDEV

Prototype `void N_VPrint_OpenMPDEV(N_Vector v)`

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

N_VPrintFile_OpenMPDEV

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

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

N_VCopyToDevice_OpenMPDEV

Prototype `void N_VCopyToDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's host data array to the device data array.

N_VCopyFromDevice_OpenMPDEV

Prototype `void N_VCopyFromDevice_OpenMPDEV(N_Vector v)`

Description This function copies the content of an NVECTOR_OPENMPDEV vector's device data array to the host data array.

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

N_VEnableFusedOps_OpenMPDEV

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

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

N_VEnableLinearCombination_OpenMPDEV

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

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

N_VEnableScaleAddMulti_OpenMPDEV

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

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

N_VEnableDotProdMulti_OpenMPDEV

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

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

N_VEnableLinearSumVectorArray_OpenMPDEV

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

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

N_VEnableScaleVectorArray_OpenMPDEV

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

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

N_VEnableConstVectorArray_OpenMPDEV

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

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

N_VEnableWrmsNormVectorArray_OpenMPDEV

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

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

N_VEnableWrmsNormMaskVectorArray_OpenMPDEV

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

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

N_VEnableScaleAddMultiVectorArray_OpenMPDEV

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

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

N_VEnableLinearCombinationVectorArray_OpenMPDEV

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

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

Notes

- When looping over the components of an N_Vector v, it is most efficient to first obtain the component array via `h_data = NV_DATA_HOST_OMPDEV(v)` for the host array or `d_data = NV_DATA_DEV_OMPDEV(v)` for the device array and then access `h_data[i]` or `d_data[i]` within the loop.

- When accessing individual components of an `N_Vector` `v` on the host remember to first copy the array back from the device with `N_VCopyFromDevice_OpenMPDEV(v)` to ensure the array is up to date.



- `N_VNewEmpty_OpenMPDEV`, `N_VMake_OpenMPDEV`, and `N_VCloneVectorArrayEmpty_OpenMPDEV` set the field `own_data = SUNFALSE`. `N_VDestroy_OpenMPDEV` and `N_VDestroyVectorArray_OpenMPDEV` will not attempt to free the pointer `data` for any `N_Vector` with `own_data` set to `SUNFALSE`. In such a case, it is the user's responsibility to deallocate the `data` pointer.



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

6.12 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.

6.12.1 NVECTOR_TRILINOS functions

The `NVECTOR_TRILINOS` module defines implementations of all vector operations listed in Tables 6.1.1, 6.1.4, and 6.1.4, 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 [30].

The names of vector operations are obtained from those in Tables 6.1.1, 6.1.4, and 6.1.4 by appending the suffix `_Trilinos` (e.g. `N_VDestroy_Trilinos`). Vector operations call existing `Tpetra::Vector` methods when available. Vector operations specific to `SUNDIALS` are implemented as standalone functions in the namespace `Sundials::TpetraVector`, located in the file `SundialsTpetraVectorKernels.hpp`. The module `NVECTOR_TRILINOS` provides the following additional user-callable functions:

- `N_VGetVector_Trilinos`

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

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

- `N_VMake_Trilinos`

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

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

Notes

- The template parameter `vector_type` should be set as:


```
typedef Sundials::TpetraVectorInterface::vector_type vector_type
```

 This will ensure that data types used in Tpetra vector match those in SUNDIALS.
- When there is a need to access components of an `N_Vector_Trilinos`, `v`, it is recommended to extract the Trilinos vector object via `x_vec = N_VGetVector_Trilinos(v)` and then access components using the appropriate Trilinos functions.
- The functions `N_VDestroy_Trilinos` and `N_VDestroyVectorArray_Trilinos` only delete the `N_Vector` wrapper. The underlying Tpetra vector object will exist for as long as there is at least one reference to it.

6.13 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:

- 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`.
- 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.

6.13.1 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.

6.13.2 NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix `_ManyVector` (e.g. `N_VDestroy_ManyVector`). The module NVECTOR_MANYVECTOR provides the following additional user-callable routines:

`N_VNew_ManyVector`

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

Description This function creates a ManyVector from a set of existing NVECTOR objects.

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

Upon successful completion, the new ManyVector is returned; otherwise this routine returns NULL (e.g., a memory allocation failure occurred).

Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions `N_VNewVectorArray`, and `N_VSetVecAtIndexVectorArray` to create the `N_Vector*` argument. This is further explained in Chapter 5.1.3.5, and the functions are documented in Chapter 6.1.5.

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 `realtypetype *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(realtypetype *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.



6.14 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:

- 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`.
- 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 6.1.4.

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.

6.14.1 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.

6.14.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, 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 6.1.1, 6.1.2, 6.1.3, and 6.1.4 by appending the suffix `_MPIManyVector` (e.g. `N_VDestroy_MPIManyVector`). The module `NVECTOR_MPIMANYVECTOR` provides the following additional user-callable routines:

`N_VNew_MPIManyVector`

Prototype `N_Vector N_VNew_MPIManyVector(sunindextype num_subvectors, N_Vector *vec_array);`

Description This function creates an `MPIManyVector` from a set of existing `NVECTOR` objects, under the requirement that all MPI-aware subvectors use the same MPI communicator (this is checked internally). If none of the subvectors are MPI-aware, then this may equivalently be used to describe data partitioning within a single node. We note that this routine is designed to support use cases A and C above.

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

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

Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions `N_VNewVectorArray`, and `N_VSetVecAtIndexVectorArray` to create the `N_Vector*` argument. This is further explained in Chapter 5.1.3.5, and the functions are documented in Chapter 6.1.5.

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 `realtpe *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(realtpe *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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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, boolean_t 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.

6.15 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.

6.15.1 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 6.14.1.

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.



6.15.2 NVECTOR_MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in Tables 6.1.1, 6.1.2, 6.1.3, and 6.1.4, from the NVECTOR_MPIMANYVECTOR (see section 6.14.2) 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, its 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.

6.16 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.

Chapter 7

Description of the SUNMatrix module

For problems that involve direct methods for solving linear systems, the SUNDIALS solvers not only operate on generic vectors, but also on generic matrices (of type `SUNMatrix`), through a set of operations defined by the particular SUNMATRIX implementation. Users can provide their own specific implementation of the SUNMATRIX module, particularly in cases where they provide their own NVECTOR and/or linear solver modules, and require matrices that are compatible with those implementations. Alternately, we provide three SUNMATRIX implementations: dense, banded, and sparse. The generic operations are described below, and descriptions of the implementations provided with SUNDIALS follow.

7.1 The SUNMatrix API

The SUNMATRIX API can be grouped into two sets of functions: the core matrix operations, and utility functions. Section 7.1.1 lists the core operations, while Section 7.1.2 lists the utility functions.

7.1.1 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 7.2.

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` (**realttype**) 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` (**realttype**) 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`

7.1.2 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`

7.1.3 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 7.1. 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 7.1: Description of the `SUNMatrix` return codes

Name	Value	Description
<code>SUNMAT_SUCCESS</code>	0	successful call or converged solve
<i>continued on next page</i>		

Table 7.2: Identifiers associated with matrix kernels supplied with SUNDIALS.

Matrix ID	Matrix type	ID Value
SUNMATRIX_DENSE	Dense $M \times N$ matrix	0
SUNMATRIX_BAND	Band $M \times M$ matrix	1
SUNMATRIX_SPARSE	Sparse (CSR or CSC) $M \times N$ 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

7.1.4 SUNMatrix identifiers

Each SUNMATRIX implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 7.2. It is recommended that a user-supplied SUNMATRIX implementation use the SUNMATRIX_CUSTOM identifier.

7.1.5 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 8. More specifically, in Table 7.3 we show the matrix interfaces available as SUNMATRIX modules, and the compatible vector implementations.

Table 7.3: SUNDIALS matrix interfaces and vector implementations that can be used for each.

Matrix Interface	Serial	Parallel (MPI)	OpenMP	pThreads	hypr Vec.	PETSc Vec.	CUDA	RAJA	User Suppl.
Dense	✓		✓	✓					✓
Band	✓		✓	✓					✓
Sparse	✓		✓	✓					✓
SLUNRloc	✓	✓	✓	✓	✓	✓			✓
User supplied	✓	✓	✓	✓	✓	✓	✓	✓	✓

7.1.6 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)(realtyp, SUNMatrix, SUNMatrix);
    int (*scaleaddi)(realtyp, 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 7.1.1 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

```

7.1.7 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 described in Section 7.1.2.

7.2 SUNMatrix functions used by CVODE

In Table 7.4, we list the matrix functions in the SUNMATRIX module used within the CVODE package. The table also shows, for each function, which of the code modules uses the function. The main CVODE 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 CVODE user does not need to know anything about the usage of matrix functions by the CVODE code modules in order to use CVODE. The information is presented as an implementation detail for the interested reader.

Table 7.4: List of matrix functions usage by CVODE code modules

	CVLS	CVBANDPRE	CVBBDPRE
<code>SUNMatGetID</code>	✓		
<code>SUNMatClone</code>	✓		
<code>SUNMatDestroy</code>	✓	✓	✓
<code>SUNMatZero</code>	✓	✓	✓
<code>SUNMatCopy</code>	✓	✓	✓
<code>SUNMatScaleAddI</code>	✓	✓	✓
<code>SUNMatSpace</code>	†	†	†

The matrix functions listed in Section 7.1.1 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 7.1.1 that are *not* used by CVODE are: SUNMatScaleAdd and SUNMatMatvec. Therefore a user-supplied SUNMATRIX module for CVODE 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.

7.3 The SUNMatrix_Dense implementation

The dense implementation of the SUNMATRIX module provided with SUNDIALS, SUNMATRIX_DENSE, defines the *content* field of SUNMatrix to be the following structure:

```
struct _SUNMatrixContent_Dense {
    sunindextype M;
    sunindextype N;
    realtype *data;
    sunindextype ldata;
    realtype **cols;
};
```

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

M - number of rows

N - number of columns

data - pointer to a contiguous block of *realtype* variables. The elements of the dense matrix are stored columnwise, i.e. the (i,j)-th element of a dense SUNMATRIX A (with $0 \leq i < M$ and $0 \leq j < N$) may be accessed via `data[j*M+i]`.

ldata - length of the data array (= M·N).

cols - array of pointers. `cols[j]` points to the first element of the j-th column of the matrix in the array `data`. The (i,j)-th element of a dense SUNMATRIX A (with $0 \leq i < M$ and $0 \leq j < N$) may be accessed via `cols[j][i]`.

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

7.3.1 SUNMatrix_Dense accessor macros

The following macros are provided to access the content of a SUNMATRIX_DENSE matrix. The prefix `SM_` in the names denotes that these macros are for *SUNMatrix* implementations, and the suffix `_D` denotes that these are specific to the *dense* version.

- `SM_CONTENT_D`

This macro gives access to the contents of the dense SUNMatrix.

The assignment `A_cont = SM_CONTENT_D(A)` sets `A_cont` to be a pointer to the dense SUNMatrix content structure.

Implementation:

```
#define SM_CONTENT_D(A) ((SUNMatrixContent_Dense)(A->content))
```

- `SM_ROWS_D`, `SM_COLUMNS_D`, and `SM_LDATA_D`

These macros give individual access to various lengths relevant to the content of a dense SUNMatrix.

These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_D(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_D(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

Implementation:

```
#define SM_ROWS_D(A)      ( SM_CONTENT_D(A)->M )
#define SM_COLUMNS_D(A)   ( SM_CONTENT_D(A)->N )
#define SM_LDATA_D(A)     ( SM_CONTENT_D(A)->ldata )
```

- `SM_DATA_D` and `SM_COLS_D`

These macros give access to the `data` and `cols` pointers for the matrix entries.

The assignment `A_data = SM_DATA_D(A)` sets `A_data` to be a pointer to the first component of the data array for the dense SUNMatrix `A`. The assignment `SM_DATA_D(A) = A_data` sets the data array of `A` to be `A_data` by storing the pointer `A_data`.

Similarly, the assignment `A_cols = SM_COLS_D(A)` sets `A_cols` to be a pointer to the array of column pointers for the dense SUNMatrix `A`. The assignment `SM_COLS_D(A) = A_cols` sets the column pointer array of `A` to be `A_cols` by storing the pointer `A_cols`.

Implementation:

```
#define SM_DATA_D(A)      ( SM_CONTENT_D(A)->data )
#define SM_COLS_D(A)     ( SM_CONTENT_D(A)->cols )
```

- `SM_COLUMN_D` and `SM_ELEMENT_D`

These macros give access to the individual columns and entries of the data array of a dense SUNMatrix.

The assignment `col_j = SM_COLUMN_D(A,j)` sets `col_j` to be a pointer to the first entry of the j -th column of the $M \times N$ dense matrix `A` (with $0 \leq j < N$). The type of the expression `SM_COLUMN_D(A,j)` is `realtypename *`. The pointer returned by the call `SM_COLUMN_D(A,j)` can be treated as an array which is indexed from 0 to $M - 1$.

The assignments `SM_ELEMENT_D(A,i,j) = a_ij` and `a_ij = SM_ELEMENT_D(A,i,j)` reference the (i,j) -th element of the $M \times N$ dense matrix `A` (with $0 \leq i < M$ and $0 \leq j < N$).

Implementation:

```
#define SM_COLUMN_D(A,j)  ( (SM_CONTENT_D(A)->cols)[j] )
#define SM_ELEMENT_D(A,i,j) ( (SM_CONTENT_D(A)->cols)[j][i] )
```

7.3.2 SUNMatrix_Dense functions

The `SUNMATRIX_DENSE` module defines dense implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix `_Dense` (e.g. `SUNMatCopy_Dense`). All the standard matrix operations listed in Section 7.1.1 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 j th column of the dense `SUNMatrix`. The resulting pointer should be indexed over the range 0 to $M - 1$.

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

Notes

- When looping over the components of a dense SUNMatrix A , the most efficient approaches are to:
 - First obtain the component array via `A_data = SM_DATA_D(A)` or `A_data = SUNDenseMatrix_Data(A)` and then access `A_data[i]` within the loop.
 - First obtain the array of column pointers via `A_cols = SM_COLS_D(A)` or `A_cols = SUNDenseMatrix_Cols(A)`, and then access `A_cols[j][i]` within the loop.
 - Within a loop over the columns, access the column pointer via `A_colj = SUNDenseMatrix_Column(A, j)` and then to access the entries within that column using `A_colj[i]` within the loop.

All three of these are more efficient than using `SM_ELEMENT_D(A, i, j)` within a double loop.

- Within the `SUNMatMatvec_Dense` routine, internal consistency checks are performed to ensure that the matrix is called with consistent NVECTOR implementations. These are currently limited to: `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS`. As additional compatible vector implementations are added to SUNDIALS, these will be included within this compatibility check.



7.3.3 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 `fsummatrix_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 fsummatrix_dense_mod`, and linking to the library `libsundials_fsummatrixdense_mod.lib` in addition to the C library. For details on where the library and module file `fsummatrix_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_fsummatrixdense_mod` library.

FORTRAN 77 interface functions

For solvers that include a FORTRAN interface module, the `SUNMATRIX_DENSE` module also includes the FORTRAN-callable function `FSUNDenseMatInit(code, M, N, ier)` to initialize this `SUNMATRIX_DENSE` module for a given SUNDIALS solver. Here `code` is an integer input solver id (1 for `CVODE`, 2 for `IDA`, 3 for `KINSOL`, 4 for `ARKODE`); `M` and `N` are the corresponding dense matrix construction arguments (declared to match C type `long int`); and `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. Additionally, when using `ARKODE` with a non-identity mass matrix, the FORTRAN-callable function `FSUNDenseMassMatInit(M, N, ier)` initializes this `SUNMATRIX_DENSE` module for storing the mass matrix.

7.4 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 7.1. A more complete description of the parts of this *content* field is given below:

M - number of rows

N - number of columns ($N = M$)

mu - upper half-bandwidth, $0 \leq \text{mu} < N$

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

s_mu - storage upper bandwidth, $\text{mu} \leq \text{s_mu} < N$. 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 $\min(N-1, \text{mu}+\text{ml})$ because of partial pivoting. The **s_mu** field holds the upper half-bandwidth allocated for A.

ldim - leading dimension ($\text{ldim} \geq \text{s_mu}+\text{ml}+1$)

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 ($= \text{ldim} \cdot N$)

cols - array of pointers. **cols[j]** is a pointer to the uppermost element within the band in the j-th column. This pointer may be treated as an array indexed from **s_mu**-**mu** (to access the uppermost element within the band in the j-th column) to **s_mu**+**ml** (to access the lowest element within the band in the j-th column). Indices from 0 to **s_mu**-**mu**-1 give access to extra storage elements required by the LU decomposition function. Finally, **cols[j][i-j+s_mu]** is the (i, j) -th element with $j-\text{mu} \leq i \leq j+\text{ml}$.

The header file to include when using this module is `sunmatrix/sunmatrix.band.h`. The SUNMATRIX_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunmatrixband` module library.

7.4.1 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) )
```

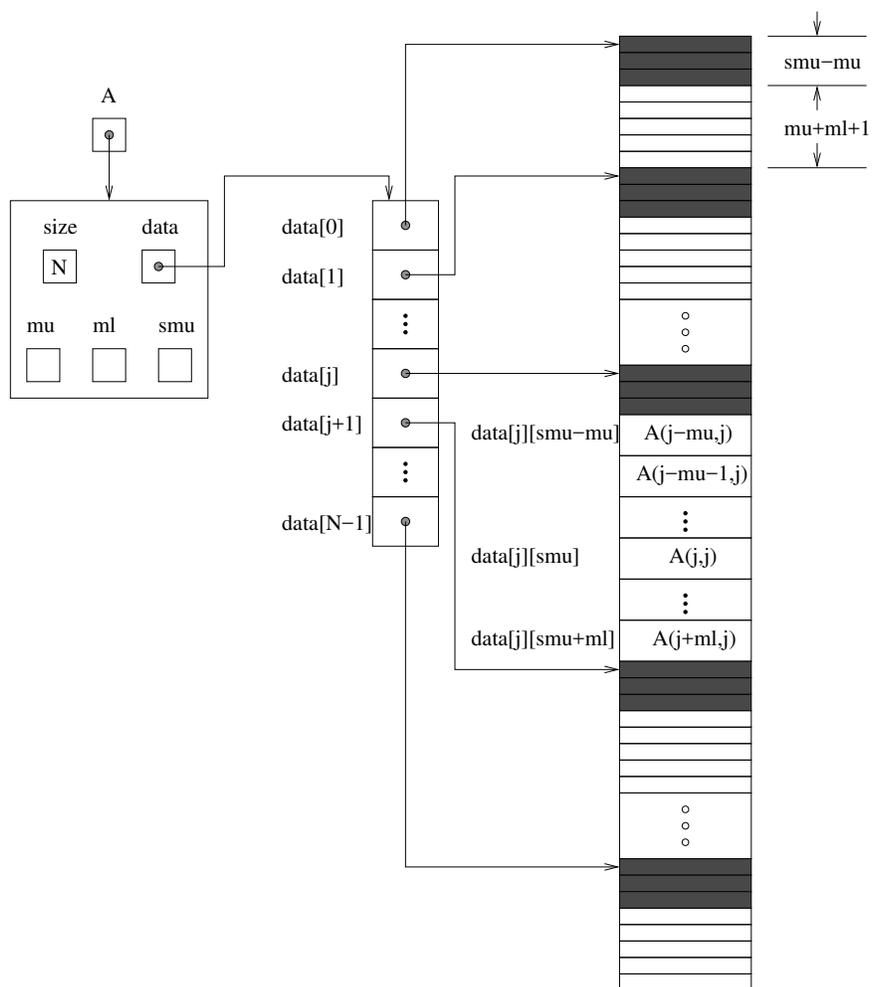


Figure 7.1: Diagram of the storage for the SUNMATRIX_BAND module. Here A is an $N \times N$ band matrix with upper and lower half-bandwidths μ and m_1 , respectively. The rows and columns of A are numbered from 0 to $N - 1$ and the (i, j) -th element of A is denoted $A(i, j)$. The greyed out areas of 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)->m1 )
#define SM_SUBAND_B(A)   ( SM_CONTENT_B(A)->s_mu )
#define SM_LDIM_B(A)     ( SM_CONTENT_B(A)->ldim )
#define SM_LDATA_B(A)    ( SM_CONTENT_B(A)->ldata )
```

- `SM_DATA_B` and `SM_COLS_B`

These macros give access to the `data` and `cols` pointers for the matrix entries.

The assignment `A_data = SM_DATA_B(A)` sets `A_data` to be a pointer to the first component of the data array for the banded SUNMatrix `A`. The assignment `SM_DATA_B(A) = A_data` sets the data array of `A` to be `A_data` by storing the pointer `A_data`.

Similarly, the assignment `A_cols = SM_COLS_B(A)` sets `A_cols` to be a pointer to the array of column pointers for the banded SUNMatrix `A`. The assignment `SM_COLS_B(A) = A_cols` sets the column pointer array of `A` to be `A_cols` by storing the pointer `A_cols`.

Implementation:

```
#define SM_DATA_B(A)      ( SM_CONTENT_B(A)->data )
#define SM_COLS_B(A)      ( SM_CONTENT_B(A)->cols )
```

- `SM_COLUMN_B`, `SM_COLUMN_ELEMENT_B`, and `SM_ELEMENT_B`

These macros give access to the individual columns and entries of the data array of a banded SUNMatrix.

The assignments `SM_ELEMENT_B(A,i,j) = a_ij` and `a_ij = SM_ELEMENT_B(A,i,j)` reference the (i,j) -th element of the $N \times N$ band matrix `A`, where $0 \leq i, j \leq N - 1$. The location (i,j) should further satisfy $j - \mu \leq i \leq j + m1$.

The assignment `col_j = SM_COLUMN_B(A,j)` sets `col_j` to be a pointer to the diagonal element of the j -th column of the $N \times N$ band matrix `A`, $0 \leq j \leq N - 1$. 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 $m1$.

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 $j - \mu \leq i \leq j + m1$.

Implementation:

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

7.4.2 SUNMatrix_Band functions

The SUNMATRIX_BAND module defines banded implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix `_Band` (e.g. `SUNMatCopy_Band`). All the standard matrix operations listed in Section 7.1.1 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 $m1$.

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.

**7.4.3 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 `f_sunmatrix_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 f_sunmatrix_band_mod`, and linking to the library `libsundials_f_sunmatrixband_mod.lib` in addition to the C library. For details on where the library and module file `f_sunmatrix_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_f_sunmatrixband_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, m1, 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 `m1` 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, m1, ier)` initializes this `SUNMATRIX_BAND` module for storing the mass matrix.

7.5 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 7.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

M - number of rows

N - number of columns

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

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

7.5.1 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.

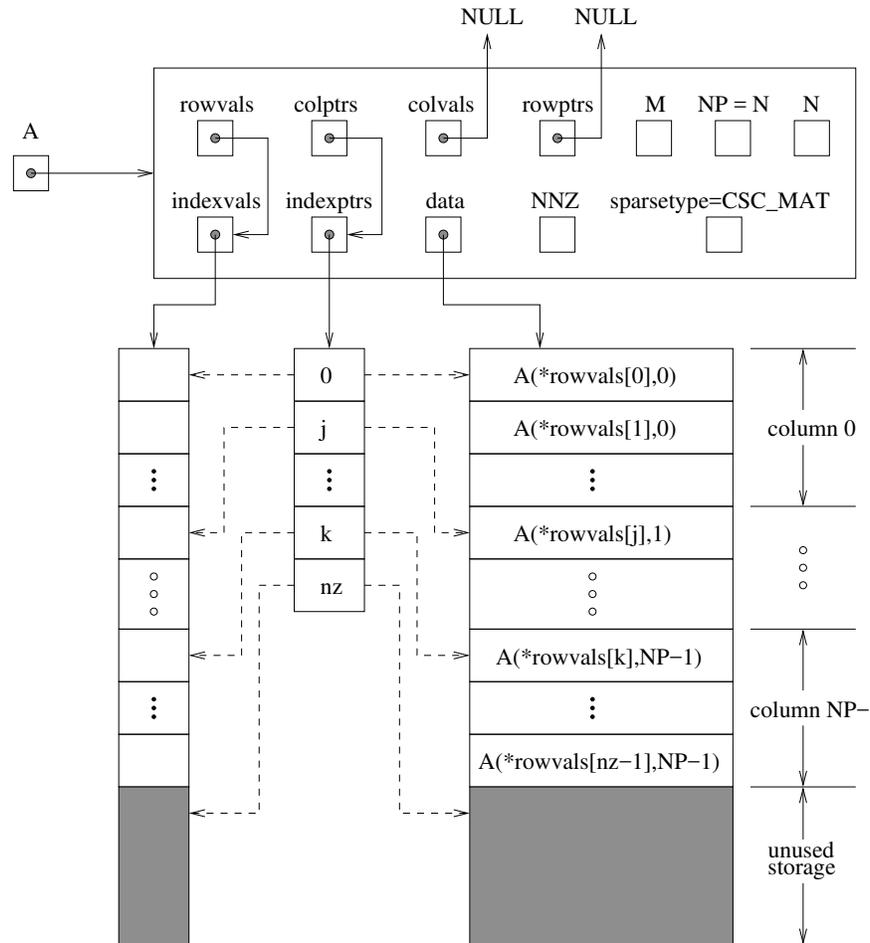


Figure 7.2: Diagram of the storage for a compressed-sparse-column matrix. Here A is an $M \times N$ sparse matrix with storage for up to NNZ nonzero entries (the allocated length of both **data** and **indexvals**). The entries in **indexvals** may assume values from 0 to $M - 1$, corresponding to the row index (zero-based) of each nonzero value. The entries in **data** contain the values of the nonzero entries, with the row i , column j entry of A (again, zero-based) denoted as $A(i, j)$. The **indexptrs** array contains $N + 1$ entries; the first N denote the starting index of each column within the **indexvals** and **data** arrays, while the final entry points one past the final nonzero entry. Here, although NNZ values are allocated, only nz are actually filled in; the greyed-out portions of **data** and **indexvals** indicate extra allocated space.

Implementation:

```
#define SM_CONTENT_S(A)      ( (SUNMatrixContent_Sparse)(A->content) )
```

- SM_ROWS_S, SM_COLUMNS_S, SM_NNZ_S, SM_NP_S, and SM_SPARSETYPE_S

These macros give individual access to various lengths relevant to the content of a sparse SUNMatrix.

These may be used either to retrieve or to set these values. For example, the assignment `A_rows = SM_ROWS_S(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_COLUMNS_S(A) = A_cols` sets the number of columns in `A` to equal `A_cols`.

Implementation:

```
#define SM_ROWS_S(A)        ( SM_CONTENT_S(A)->M )
#define SM_COLUMNS_S(A)    ( SM_CONTENT_S(A)->N )
#define SM_NNZ_S(A)        ( SM_CONTENT_S(A)->NNZ )
#define SM_NP_S(A)         ( SM_CONTENT_S(A)->NP )
#define SM_SPARSETYPE_S(A) ( SM_CONTENT_S(A)->sparsetype )
```

- SM_DATA_S, SM_INDEXVALS_S, and SM_INDEXPTRS_S

These macros give access to the `data` and `index` arrays for the matrix entries.

The assignment `A_data = SM_DATA_S(A)` sets `A_data` to be a pointer to the first component of the data array for the sparse SUNMatrix `A`. The assignment `SM_DATA_S(A) = A_data` sets the data array of `A` to be `A_data` by storing the pointer `A_data`.

Similarly, the assignment `A_indexvals = SM_INDEXVALS_S(A)` sets `A_indexvals` to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix `A`. The assignment `A_indexptrs = SM_INDEXPTRS_S(A)` sets `A_indexptrs` to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).

Implementation:

```
#define SM_DATA_S(A)        ( SM_CONTENT_S(A)->data )
#define SM_INDEXVALS_S(A)  ( SM_CONTENT_S(A)->indexvals )
#define SM_INDEXPTRS_S(A)  ( SM_CONTENT_S(A)->indexptrs )
```

7.5.2 SUNMatrix_Sparse functions

The `SUNMATRIX_SPARSE` module defines sparse implementations of all matrix operations listed in Section 7.1.1. Their names are obtained from those in Section 7.1.1 by appending the suffix `_Sparse` (e.g. `SUNMatCopy_Sparse`). All the standard matrix operations listed in Section 7.1.1 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.

7.5.3 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.

7.6 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, 23, 37, 38]. It is designed to be used with the SUNLINSOL_SUPERLUDIST linear solver discussed in Section 8.10. To this end, it defines the *content* field of SUNMatrix to be the following structure:

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

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

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

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

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

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

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

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

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

7.6.1 SUNMatrix_SLUNRloc functions

The module SUNMATRIX_SLUNRLOC provides the following user-callable routines:

<code>SUNMatrix_SLUNRloc</code>	
Call	<code>A = SUNMatrix_SLUNRloc(Asuper, grid);</code>
Description	The function <code>SUNMatrix_SLUNRloc</code> creates and allocates memory for a SUNMATRIX_SLUNRLOC object.
Arguments	<code>Asuper</code> (<code>SuperMatrix*</code>) a fully-allocated SuperLU_DIST SuperMatrix that the SUNMatrix will wrap; must have <code>Stype</code> = SLU_NR_loc, <code>Dtype</code> = SLU_D, <code>Mtype</code> = SLU_GE to be compatible <code>grid</code> (<code>gridinfo_t*</code>) the initialized SuperLU_DIST 2D process grid structure
Return value	a SUNMatrix object if <code>Asuper</code> 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 7.1.1:

- `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.



7.7 The SUNMatrix_cuSparse implementation

The `SUNMATRIX_CUSPARSE` implementation of the `SUNMatrix` module provided with SUNDIALS, is an interface to the NVIDIA cuSPARSE matrix for use on NVIDIA GPUs [?]. All data stored by this matrix implementation resides on the GPU at all times. The implementation currently supports the cuSPARSE CSR matrix format described in the cuSPARSE documentation as well as a unique low-storage format for block-diagonal matrices of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{A}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A}_n \end{bmatrix}$$

where all the block matrices A_j share the same sparsity pattern. We will refer to this format as BCSR (not to be confused with the canonical BSR format where each block is stored as dense). In this format, the CSR column indices and row pointers are only stored for the first block and are computed only as necessary for other blocks. This can drastically reduce the amount of storage required compared to the regular CSR format when there is a large number of blocks. This format is well-suited for, and intended to be used with the 8.12.

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

The `SUNMatrix_cuSparse` module is experimental and subject to change.



7.7.1 SUNMatrix_cuSparse functions

The `SUNMATRIX_CUSPARSE` module defines GPU-enabled sparse implementations of all matrix operations listed in the section :ref:'SUNMatrix.Ops' except for the “`SUNMatSpace`“ and “`SUNMatMatvecSetup`“ operations:

1. `SUNMatGetID_cuSparse` – returns `SUNMATRIX_CUSPARSE`
2. `SUNMatClone_cuSparse`
3. `SUNMatDestroy_cuSparse`
4. `SUNMatZero_cuSparse`
5. `SUNMatCopy_cuSparse`
6. `SUNMatScaleAdd_cuSparse` – performs $A = cA + B$, where A and B must have the same sparsity pattern

7. `SUNMatScaleAddI_cuSparse` – performs $A = cA + I$, where the diagonal of A must be present
8. `SUNMatMatvec_cuSparse`

In addition, the `SUNMATRIX_CUSPARSE` module defines the following implementation specific functions:

`SUNMatrix_cuSparse_NewCSR`

Call `A = SUNMatrix_cuSparse_NewCSR(M, N, NNZ, cusp)`

Description This constructor function creates and allocates memory for a `SUNMATRIX_CUSPARSE` `SUNMatrix` that uses the CSR storage format.

Arguments `M` (`int`) the number of matrix rows
`N` (`int`) the number of matrix columns
`NNZ` (`int`) the number of matrix nonzeros
`cusp` (`cusparseHandle_t`) a valid `cusparseHandle_t`

Return value a `SUNMatrix` object if successful else `NULL`

Notes

`SUNMatrix_cuSparse_NewBlockCSR`

Call `A = SUNMatrix_cuSparse_NewBlockCSR(nblocks, blockrows, blockcols, blocknnz, cusp)`

Description This constructor function creates and allocates memory for a `SUNMATRIX_CUSPARSE` `SUNMatrix` that leverages the `SUNMAT_CUSPARSE_BCSR` storage format to store a block diagonal matrix where each block shares the same sparsity pattern. **The blocks must be square.**

Arguments `nblocks` (`int`) the number of matrix blocks
`blockrows` (`int`) the number of rows for a block
`blockcols` (`int`) the number of columns for a block
`blocknnz` (`int`) the number of nonzeros in a block
`cusp` a valid `cusparseHandle_t`

Return value a `SUNMatrix` object if successful else `NULL`

Notes The `SUNMAT_CUSPARSE_BCSR` format currently only supports square matrices.

`SUNMatrix_cuSparse_MakeCSR`

Call `A = SUNMatrix_cuSparse_MakeCSR(mat_descr, M, N, NNZ, rowptrs, colind, data, cusp)`

Description This constructor function creates and allocates memory for a `SUNMATRIX_CUSPARSE` `SUNMatrix` that uses the CSR storage format from the user provided pointers.

Arguments `mat_descr` a valid `cusparseMatDescr_t` object; must use `CUSPARSE_INDEX_BASE_ZERO` indexing
`M` (`int`) the number of matrix rows
`N` (`int`) the number of matrix columns
`NNZ` (`int`) the number of matrix nonzeros
`rowptrs` (`int*`) a contiguous array of the CSR row pointers
`colind` (`int*`) a contiguous array of the CSR column indices
`data` (`realtype*`) a contiguous array of the nonzero data
`cusp` (`cusparseHandle_t`) a valid `cusparseHandle_t`

Return value a `SUNMatrix` object if successful else `NULL`

Notes

SUNMatrix_cuSparse_Rows

Call `M = SUNMatrix_cuSparse_Rows(A)`

Description This function returns the number of rows in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of rows in the sparse `SUNMatrix`

Notes

SUNMatrix_cuSparse_Columns

Call `N = SUNMatrix_cuSparse_Columns(A)`

Description This function returns the number of columns in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of columns in the sparse `SUNMatrix`

Notes

SUNMatrix_cuSparse_NNZ

Call `nnz = SUNMatrix_cuSparse_NNZ(A)`

Description This function returns the number of nonzeros in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of nonzeros in the sparse `SUNMatrix`

Notes

SUNMatrix_cuSparse_SparseType

Call `type = SUNMatrix_cuSparse_SparseType(A)`

Description This function returns the sparsity format for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the `SUNMAT_CUSPARSE_CSR` or `SUNMAT_CUSPARSE_BCSR` sparsity formats

Notes

SUNMatrix_cuSparse_IndexValues

Call `colind = SUNMatrix_cuSparse_IndexValues(A)`

Description This function returns a pointer to the index value array for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value for the CSR format this is an array of the column indices for each nonzero entry. For the BCSR format this is an array of the column indices for each nonzero entry in the first block only.

Notes

`SUNMatrix_cuSparse_IndexPointers`

Call `rowptrs = SUNMatrix_cuSparse_IndexPointers(A)`

Description This function returns a pointer to the index pointers array for the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value for the CSR format this is an array of the locations of the first entry of each row in the `data` and `indexvalues` arrays, for the BCSR format this is an array of the locations of each row in the `data` and `indexvalues` arrays in the first block only.

Notes

`SUNMatrix_cuSparse_NumBlocks`

Call `nblocks = SUNMatrix_cuSparse_NumBlocks(A)`

Description This function returns the number of blocks in the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of matrix blocks

Notes

`SUNMatrix_cuSparse_BlockRows`

Call `blockrows = SUNMatrix_cuSparse_BlockRows(A)`

Description This function returns the number of rows of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of rows of a block

Notes

`SUNMatrix_cuSparse_BlockColumns`

Call `blockrows = SUNMatrix_cuSparse_BlockColumns(A)`

Description This function returns the number of columns of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of columns of a block

Notes

`SUNMatrix_cuSparse_BlockNNZ`

Call `blockdim = SUNMatrix_cuSparse_BlockNNZ(A)`

Description This function returns the nonzeros of a block of the sparse `SUNMatrix`.

Arguments `A` (`SUNMatrix`)

Return value the number of nonzeros of a block

Notes

SUNMatrix_cuSparse_BlockData

Call `nzdata = SUNMatrix_cuSparse_BlockData(A, blockidx)`

Description This function returns a pointer to the start of the nonzero values in the data array for given block index. The first block in the `SUNMatrix` is index 0, the second block is index 1, and so on.

Arguments `A` (`SUNMatrix`)
`blockidx` (`int`) the index of the desired block

Return value a pointer to the start of the nonzero values in the data array for given block index

Notes

SUNMatrix_cuSparse_CopyToDevice

Call `retval = SUNMatrix_cuSparse_CopyToDevice(A, h_data, h_idxptrs, h_idxvals)`

Description This functions copies the matrix information to the GPU device from the provided host arrays. A user may provide `NULL` for any of `h_data`, `h_idxptrs`, or `h_idxvals` to avoid copying that information.

Arguments `A` (`SUNMatrix`)
`h_data` (`realtyp*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_NNZ(A)*sizeof(realtyp)` bytes; the nonzero values will be copied from this array onto the device
`h_idxptrs` (`int*`) a pointer to an allocated array of at least `(SUNMatrix_cuSparse_BlockDim(A)+1)*sizeof(int)` bytes; the index pointers will be copied from this array onto the device
`h_idxvals` (`int*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_BlockNNZ(A)*sizeof(int)` bytes; the index values will be copied from this array onto the device

Return value `SUNMAT_SUCCESS` if the copy operation(s) were successful, or a nonzero error code otherwise.

Notes

SUNMatrix_cuSparse_CopyFromDevice

Call `retval = SUNMatrix_cuSparse_CopyFromDevice(A, h_data, h_idxptrs, h_idxvals)`

Description This functions copies the matrix information from the GPU device to the provided host arrays. A user may provide `NULL` for any of `h_data`, `h_idxptrs`, or `h_idxvals` to avoid copying that information.

Arguments `A` (`SUNMatrix`)
`h_data` (`realtyp*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_NNZ(A)*sizeof(realtyp)` bytes; the nonzero values will be copied into this array from the device
`h_idxptrs` (`int*`) a pointer to an allocated array of at least `(SUNMatrix_cuSparse_BlockDim(A)+1)*sizeof(int)` bytes; the index pointers will be copied into this array from the device
`h_idxvals` (`int*`) a pointer to an allocated array of at least `SUNMatrix_cuSparse_BlockNNZ(A)*sizeof(int)` bytes; the index values will be copied into this array from the device

Return value `SUNMAT_SUCCESS` if the copy operation(s) were successful, or a nonzero error code otherwise.

Notes

SUNMatrix_cuSparse_SetFixedPattern

Call `retval = SUNMatrix_cuSparse_SetFixedPattern(A, yesno)`

Description This function changes the behavior of the the `SUNMatZero` operation on the `SUNMatrix` object `A`. By default the matrix sparsity pattern is not considered to be fixed, thus, the `SUNMatZero` operation zeros out all `data` array as well as the `indexvalues` and `indexpointers` arrays. Providing a value of 1 or `SUNTRUE` for the `yesno` argument changes the behavior of `SUNMatZero` on `A` so that only the data is zeroed out, but not the `indexvalues` or `indexpointers` arrays. Providing a value of 0 or `SUNFALSE` for the `yesno` argument is equivalent to the default behavior.

Arguments `A` (`SUNMatrix`)
`yesno` (`booleantype`)

Return value `SUNMAT_SUCCESS` if the operation(s) were successful, or a nonzero error code otherwise.

Notes

7.7.2 `SUNMatrix_cuSparse` Usage Notes

The `SUNMATRIX_CUSPARSE` module only supports 32-bit indexing, thus `SUNDIALS` must be built for 32-bit indexing to use this module.

The `SUNMATRIX_CUSPARSE` module can be used with `CUDA` streams by calling the `cuSPARSE` function `cusparseSetStream` on the the `cusparseHandle_t` that is provided to the `SUNMATRIX_CUSPARSE` constructor.



When using the `SUNMATRIX_CUSPARSE` module with a `SUNDIALS` package (e.g. `CVODE`), the stream given to `cuSPARSE` should be the same stream used for the `NVECTOR` object that is provided to the package, and the `NVECTOR` object given to the `SUNMatvec` operation. If different streams are utilized, synchronization issues may occur.

Chapter 8

Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS packages operate using generic linear solver modules defined through the SUNLINSOL API. This allows SUNDIALS packages to utilize any valid SUNLINSOL implementation that provides a set of required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group consists of “set” routines to supply the linear solver object with functions provided by the SUNDIALS package, or for modification of solver parameters. The last group consists of “get” routines for retrieving artifacts (statistics, residual vectors, etc.) from the linear solver. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

The implementations provided with SUNDIALS work in coordination with the SUNDIALS generic NVECTOR and SUNMATRIX modules to provide a set of compatible data structures and solvers for the solution of linear systems using direct or iterative (matrix-based or matrix-free) methods. Moreover, advanced users can provide a customized `SUNLinearSolver` implementation to any SUNDIALS package, particularly in cases where they provide their own NVECTOR and/or SUNMATRIX modules.

Historically, the SUNDIALS packages have been designed to specifically leverage the use of either *direct linear solvers* or matrix-free, *scaled, preconditioned, iterative linear solvers*. However, matrix-based iterative linear solvers are also supported.

The iterative linear solvers packaged with SUNDIALS leverage scaling and preconditioning, as applicable, to balance error between solution components and to accelerate convergence of the linear solver. To this end, instead of solving the linear system $Ax = b$ directly, these apply the underlying iterative algorithm to the transformed system

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

where

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

and where

- P_1 is the left preconditioner,
- P_2 is the right preconditioner,
- S_1 is a diagonal matrix of scale factors for $P_1^{-1}b$,
- S_2 is a diagonal matrix of scale factors for P_2x .

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

SUNDIALS packages request that iterative linear solvers stop based on the 2-norm of the scaled preconditioned residual meeting a prescribed tolerance

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

When provided an iterative SUNLINSOL implementation that does not support the scaling matrices S_1 and S_2 , SUNDIALS' packages will adjust the value of tol accordingly (see §8.4.2 for more details). In this case, they instead request that iterative linear solvers stop based on the criteria

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

We note that the corresponding adjustments to tol in this case are non-optimal, in that they cannot balance error between specific entries of the solution x , only the aggregate error in the overall solution vector.

We further note that not all of the SUNDIALS-provided iterative linear solvers support the full range of the above options (e.g., separate left/right preconditioning), and that some of the SUNDIALS packages only utilize a subset of these options. Further details on these exceptions are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS package.

For users interested in providing their own SUNLINSOL module, the following section presents the SUNLINSOL API and its implementation beginning with the definition of SUNLINSOL functions in sections 8.1.1 – 8.1.3. This is followed by the definition of functions supplied to a linear solver implementation in section 8.1.4. A table of linear solver return codes is given in section 8.1.5. The `SUNLinearSolver` type and the generic SUNLINSOL module are defined in section 8.1.6. The section 8.2 discusses compatibility between the SUNDIALS-provided SUNLINSOL modules and SUNMATRIX modules. Section 8.3 lists the requirements for supplying a custom SUNLINSOL module and discusses some intended use cases. Users wishing to supply their own SUNLINSOL module are encouraged to use the SUNLINSOL implementations provided with SUNDIALS as a template for supplying custom linear solver modules. The SUNLINSOL functions required by this SUNDIALS package as well as other package specific details are given in section 8.4. The remaining sections of this chapter present the SUNLINSOL modules provided with SUNDIALS.

8.1 The SUNLinearSolver API

The SUNLINSOL API defines several linear solver operations that enable SUNDIALS packages to utilize any SUNLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core linear solver functions. The second group of functions consists of set routines to supply the linear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving linear solver statistics. All of these functions are defined in the header file `sundials/sundials_linearsolver.h`.

8.1.1 SUNLinearSolver core functions

The core linear solver functions consist of 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 8.3.1 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 8.1.

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 8.1.

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 8.1.

Notes **Direct solvers:** can ignore the `tol` argument.

Matrix-free solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE`) can ignore the SUNMATRIX input `A`, and should instead rely on the matrix-vector product function supplied through the routine `SUNLinSolSetATimes`.

Iterative solvers: (those that identify as `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`) should attempt to solve to the specified tolerance `tol` in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.

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`

8.1.2 SUNLinearSolver set functions

The following set functions are used to supply linear solver modules with functions defined by the SUNDIALS packages and to modify solver parameters. Only the routine for setting the matrix-vector product routine is required, and that is only for matrix-free linear solver modules. Otherwise, all other set functions are optional. SUNLINSOL implementations that do not provide the functionality for any optional routine should leave the corresponding function pointer NULL instead of supplying a dummy routine.

SUNLinSolSetATimes

Call `retval = SUNLinSolSetATimes(LS, A_data, ATimes);`

Description The function `SUNLinSolSetATimes` is *required for matrix-free linear solvers*; otherwise it is optional.

This routine provides an `ATimesFn` function pointer, as well as a `void*` pointer to a data structure used by this routine, to a linear solver object. SUNDIALS packages will call this function to set the matrix-vector product function to either a solver-provided difference-quotient via vector operations or a user-supplied solver-specific routine.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`A_data` (`void*`) data structure passed to `ATimes`.
`ATimes` (`ATimesFn`) function pointer implementing the matrix-vector product routine.

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 8.1.

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 (8.1)-(8.2). This routine will be called by a SUNDIALS package, which will provide translation between the generic `Pset` and `Psol` calls and the package- or user-supplied routines.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`Pdata` (`void*`) data structure passed to both `Pset` and `Psol`.
`Pset` (`PSetupFn`) function pointer implementing the preconditioner setup.
`Psol` (`PSolveFn`) function pointer implementing the preconditioner solve.

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 8.1.

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 (8.1)-(8.2), respectively. Neither of these vectors need to be tested for positivity, and a `NULL` argument for either indicates that the corresponding scaling matrix is the identity.

Arguments `LS` (`SUNLinearSolver`) a SUNLINSOL object.
`s1` (`NVECTOR`) diagonal of the matrix S_1

s2 (`N_Vector`) diagonal of the matrix S_2

Return value This routine should return zero for a successful call, and a negative value for a failure, ideally returning one of the generic error codes listed in Table 8.1.

F2003 Name FSUNLinSolSetScalingVectors

8.1.3 SUNLinearSolver get functions

The following get functions allow SUNDIALS packages to retrieve results from a linear solve. All routines are optional.

SUNLinSolNumIters

Call `its = SUNLinSolNumIters(LS);`

Description The *optional* function `SUNLinSolNumIters` should return the number of linear iterations performed in the last ‘solve’ call.

Arguments `LS` (`SUNLinearSolver`) a `SUNLINSOL` object.

Return value `int` containing the number of iterations

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 8.1.

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

F2003 Name `FSUNLinSolSpace`

8.1.4 Functions provided by SUNDIALS packages

To interface with the `SUNLINSOL` modules, the `SUNDIALS` packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic interfaces to the linear systems of equations that result in their solution. The types for functions provided to a `SUNLINSOL` module are defined in the header file `sundials/sundials_iterative.h`, and are described below.

ATimesFn

Definition `typedef int (*ATimesFn)(void *A_data, N_Vector v, N_Vector z);`

Purpose These functions compute the action of a matrix on a vector, performing the operation $z = Av$. Memory for `z` should already be allocated 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.

Name	Value	Description
SUNLS_PSET_FAIL_UNREC	-805	an unrecoverable failure occurred in the <code>Pset</code> routine
SUNLS_PSOLVE_FAIL_UNREC	-806	an unrecoverable failure occurred in the <code>Psolve</code> 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_SPGMR)
SUNLS_QRSOL_FAIL	-809	a singular R matrix was encountered in a QR factorization (SUNLINSOL_SPGMR/SUNLINSOL_SPGMR)
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_ATHES_FAIL_REC	803	a recoverable failure occurred in the <code>ATimes</code> routine
SUNLS_PSET_FAIL_REC	804	a recoverable failure occurred in the <code>Pset</code> routine
SUNLS_PSOLVE_FAIL_REC	805	a recoverable failure occurred in the <code>Psolve</code> 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_SPGMR)
SUNLS_LUFACT_FAIL	808	a singular matrix was encountered during a LU factorization (SUNLINSOL_DENSE/SUNLINSOL_BAND)

8.1.6 The generic SUNLinearSolver module

SUNDIALS packages interact with specific SUNLINSOL implementations through the generic SUNLINSOL module on which all other SUNLINSOL implementations 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 8.1.1-8.1.3. These routines are in fact only wrappers to the linear solver operations defined by a particular SUNLINSOL implementation, which are accessed through the *ops* field of the SUNLinearSolver structure. To illustrate this point we show below the implementation of a typical linear solver operation from the generic SUNLINSOL module, namely SUNLinSolInitialize, which initializes a SUNLINSOL object for use after it has been created and configured, and returns a flag denoting a successful/failed operation:

```

int SUNLinSolInitialize(SUNLinearSolver S)
{
  return ((int) S->ops->initialize(S));
}

```

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

```

8.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 8.2 we show the matrix-based linear solvers available as SUNLINSOL modules, and the compatible matrix implementations. Recall that Table 4.1 shows the compatibility between all SUNLINSOL modules and vector implementations.

Table 8.2: SUNDIALS matrix-based linear solvers and matrix implementations that can be used for each.

Linear Solver Interface	Dense Matrix	Banded Matrix	Sparse Matrix	SLUNRloc Matrix	User Supplied
Dense	✓				✓
Band		✓			✓
LapackDense	✓				✓
LapackBand		✓			✓
KLU			✓		✓
SuperLU_DIST				✓	✓
SUPERLUMT			✓		✓
User supplied	✓	✓	✓	✓	✓

8.3 Implementing a custom SUNLinearSolver module

A particular implementation of the SUNLINSOL module must:

- Specify the *content* field of the SUNLinearSolver object.
- Define and implement a minimal subset of the linear solver operations. See the section 8.4 to determine which SUNLINSOL operations are required for this SUNDIALS package.

Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNLINSOL module (each with different SUNLinearSolver internal data representations) in the same code.

- Define and implement user-callable constructor and destructor routines to create and free a SUNLinearSolver with the new *content* field and with *ops* pointing to the new linear solver operations.

We note that the function pointers for all unsupported optional routines should be set to `NULL` in the *ops* structure. This allows the SUNDIALS package that is using the SUNLINSOL object to know that the associated functionality is not supported.

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.

8.3.1 Intended use cases

The `SUNLINSOL` (and `SUNMATRIX`) APIs are designed to require a minimal set of routines to ease interfacing with custom or third-party linear solver libraries. External solvers provide similar routines with the necessary functionality and thus will require minimal effort to wrap within custom `SUNMATRIX` and `SUNLINSOL` implementations. Sections 7.2 and 8.4 include a list of the required set of routines that compatible `SUNMATRIX` and `SUNLINSOL` implementations must provide. As `SUNDIALS` packages utilize generic `SUNLINSOL` modules allowing for user-supplied `SUNLinearSolver` implementations, there exists a wide range of possible linear solver combinations. Some intended use cases for both the `SUNDIALS`-provided and user-supplied `SUNLINSOL` modules are discussed in the following sections.

Direct linear solvers

Direct linear solver modules require a matrix and compute an ‘exact’ solution to the linear system *defined by the matrix*. Multiple matrix formats and associated direct linear solvers are supplied with `SUNDIALS` through different `SUNMATRIX` and `SUNLINSOL` implementations. `SUNDIALS` packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations. As a result, each package’s linear solver interface recomputes Jacobian information as infrequently as possible.

Alternative matrix storage formats and compatible linear solvers that are not currently provided by, or interfaced with, `SUNDIALS` can leverage this infrastructure with minimal effort. To do so, a user must implement custom `SUNMATRIX` and `SUNLINSOL` wrappers for the desired matrix format and/or linear solver following the APIs described in Chapters 7 and 8. *This user-supplied `SUNLINSOL` module must then self-identify as having `SUNLINEARSOLVER_DIRECT` type.*

Matrix-free iterative linear solvers

Matrix-free iterative linear solver modules do not require a matrix and compute an inexact solution to the linear system *defined by the package-supplied `ATimes` routine*. `SUNDIALS` supplies multiple scaled, preconditioned iterative linear solver (spils) `SUNLINSOL` modules that support scaling to allow users to handle non-dimensionalization (as best as possible) within each `SUNDIALS` package and retain variables and define equations as desired in their applications. For linear solvers that do not support left/right scaling, the tolerance supplied to the linear solver is adjusted to compensate (see section 8.4.2 for more details); however, this use case may be non-optimal and cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single problem.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, `SUNDIALS` a user must implement a custom `SUNLINSOL` wrapper for the linear solver following the API described in Chapter 8. *This user-supplied `SUNLINSOL` module must then self-identify as having `SUNLINEARSOLVER_ITERATIVE` type.*

Matrix-based iterative linear solvers (reusing A)

Matrix-based iterative linear solver modules require a matrix and compute an inexact solution to the linear system *defined by the matrix*. This matrix will be updated infrequently and reused 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 *hypr* library that may be used as a template for other customized implementations (see `examples/arkode/CXX_parhyp/ark_heat2D_hypr.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_SPGFMR`, `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.

8.4 CVODE SUNLinearSolver interface

Table 8.3 below lists the SUNLINSOL module linear solver functions used within the CVLS interface. As with the SUNMATRIX module, we emphasize that the CVODE user does not need to know detailed usage of linear solver functions by the CVODE code modules in order to use CVODE. 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 8.3: 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	†	†	†

8.4.1 Lagged matrix information

If the SUNLINSOL object self-identifies as having type `SUNLINEARSOLVER_DIRECT` or `SUNLINEARSOLVER_MATRIX_ITERATIVE`, then the SUNLINSOL object solves a linear system *defined* by a SUNMATRIX object. CVLS will update the matrix information infrequently according to the strategies outlined in §2.1. 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

$$x = \frac{2}{1 + \gamma/\bar{\gamma}}\bar{x}. \quad (8.3)$$

The motivation for this selection of the scaling factor $c = 2/(1 + \gamma/\bar{\gamma})$ is discussed in detail in [8, 28]. 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 .

8.4.2 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

$$W_i \approx W_{mean}, \quad \text{for } i = 0, \dots, n-1.$$

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 (8.1)-(8.2)):

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

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2 / \sqrt{n}$$

is computed and the scaled tolerance `delta = tol/Wmean` is supplied to the SUNLINSOL object.

8.5 The SUNLinearSolver_Dense implementation

This section describes the SUNLINSOL implementation for solving dense linear systems. The SUNLINSOL_DENSE module is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

To access the SUNLINSOL_DENSE module, include the header file `sunlinsol/sunlinsol_dense.h`. We note that the SUNLINSOL_DENSE module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsoldense` module library.

8.5.1 SUNLinearSolver_Dense description

This solver is constructed to perform the following operations:

- The “setup” call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1’s on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A , with pivoting information encoding P stored in the `pivots` array.
- The “solve” call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

8.5.2 SUNLinearSolver_Dense functions

The SUNLINSOL_DENSE module provides the following user-callable constructor for creating a SUNLinearSolver object.

<code>SUNLinSol_Dense</code>	
Call	<code>LS = SUNLinSol_Dense(y, A);</code>
Description	The function <code>SUNLinSol_Dense</code> creates and allocates memory for a dense <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>A</code> (<code>SUNMatrix</code>) a <code>SUNMATRIX_DENSE</code> matrix template for cloning matrices needed within the solver
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_DENSE</code> matrix type and the <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> , and <code>NVECTOR_PTHREADS</code> vector types. As additional compatible matrix and vector implementations are added to <code>SUNDIALS</code> , these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function <code>SUNDenseLinearSolver</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_Dense</code>

The `SUNLINSOL_DENSE` module defines implementations of all “direct” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_Dense`
- `SUNLinSolInitialize_Dense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_Dense` – this performs the *LU* factorization.
- `SUNLinSolSolve_Dense` – this uses the *LU* factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_Dense`
- `SUNLinSolSpace_Dense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_Dense`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

8.5.3 SUNLinearSolver_Dense Fortran interfaces

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

FORTTRAN 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(<i>code</i> , <i>ier</i>)
Description	The function FSUNDENSELINSOLINIT can be called for Fortran programs to create a dense SUNLinearSolver object.
Arguments	<i>code</i> (<i>int*</i>) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
Return value	<i>ier</i> 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 <i>after</i> 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(<i>ier</i>)
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	<i>ier</i> is a <i>int</i> 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 <i>after</i> both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

8.5.4 SUNLinearSolver_Dense content

The SUNLINSOL_DENSE module defines the *content* field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_Dense {
    sunindextype N;
    sunindextype *pivots;
    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.

8.6 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.

8.6.1 SUNLinearSolver_Band description

This solver is constructed to perform the following operations:

- The “setup” call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1’s on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A , with pivoting information encoding P stored in the `pivots` array.
- The “solve” call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_BAND object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `m1`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1, mu+m1)`. The lower triangular factor L has lower bandwidth `m1`.



8.6.2 SUNLinearSolver_Band functions

The SUNLINSOL_BAND module provides the following user-callable constructor for creating a SUNLinearSolver object.

<code>SUNLinSol_Band</code>	
Call	<code>LS = SUNLinSol_Band(y, A);</code>
Description	The function <code>SUNLinSol_Band</code> creates and allocates memory for a band <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>A</code> (<code>SUNMatrix</code>) a <code>SUNMATRIX_BAND</code> matrix template for cloning matrices needed within the solver
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_BAND</code> matrix type and the <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> , and <code>NVECTOR_PTHREADS</code> 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 <code>A</code> is allocated with appropriate upper bandwidth storage for the LU factorization.
Deprecated Name	For backward compatibility, the wrapper function <code>SUNBandLinearSolver</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_Band</code>

The SUNLINSOL_BAND module defines band implementations of all “direct” linear solver operations listed in Sections [8.1.1](#) – [8.1.3](#):

- `SUNLinSolGetType_Band`
- `SUNLinSolInitialize_Band` – this does nothing, since all consistency checks are performed at solver creation.

- `SUNLinSolSetup_Band` – this performs the LU factorization.
- `SUNLinSolSolve_Band` – this uses the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_Band`
- `SUNLinSolSpace_Band` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_Band`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

8.6.3 SUNLinearSolver_Band Fortran interfaces

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

FORTRAN 2003 interface module

The `fsunlinsol_band_mod` FORTRAN module defines interfaces to all `SUNLINSOL_BAND` C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading ‘F’. For example, the function `SUNLinSol_Band` is interfaced as `FSUNLinSol_Band`.

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the `SUNLINSOL_BAND` module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNBANDLINSOLINIT

Call	<code>FSUNBANDLINSOLINIT(code, ier)</code>
Description	The function <code>FSUNBANDLINSOLINIT</code> can be called for Fortran programs to create a band <code>SUNLinearSolver</code> object.
Arguments	<code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for <code>CVODE</code> , 2 for <code>IDA</code> , 3 for <code>KINSOL</code> , and 4 for <code>ARKODE</code>).
Return value	<code>ier</code> 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 <i>after</i> both the <code>NVECTOR</code> and <code>SUNMATRIX</code> 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(<i>ier</i>)
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	<i>ier</i> is a <code>int</code> 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 <i>after</i> both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

8.6.4 SUNLinearSolver_Band content

The SUNLINSOL_BAND module defines the *content* field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_Band {
    sunindextype N;
    sunindextype *pivots;
    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.

8.7 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 `realtyp` 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 `realtyp`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLINSOL_LAPACKDENSE module also cannot be compiled when using 64-bit integers for the `sunindextype`.



8.7.1 SUNLinearSolver_LapackDense description

This solver is constructed to perform the following operations:

- The “setup” call performs a LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1’s on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A , with pivoting information encoding P stored in the `pivots` array.
- The “solve” call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

8.7.2 SUNLinearSolver_LapackDense functions

The SUNLINSOL_LAPACKDENSE module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_LapackDense

Call	<code>LS = SUNLinSol_LapackDense(y, A);</code>
Description	The function <code>SUNLinSol_LapackDense</code> creates and allocates memory for a LAPACK-based, dense <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>A</code> (<code>SUNMatrix</code>) a SUNMATRIX_DENSE matrix template for cloning matrices needed within the solver
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_DENSE</code> matrix type and the <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> , and <code>NVECTOR_PTHREADS</code> vector types. As additional compatible matrix and vector implementations are added to <code>SUNDIALS</code> , these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function <code>SUNLapackDense</code> with identical input and output arguments is also provided.

The SUNLINSOL_LAPACKDENSE module defines dense implementations of all “direct” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_LapackDense`
- `SUNLinSolInitialize_LapackDense` – this does nothing, since all consistency checks are performed at solver creation.
- `SUNLinSolSetup_LapackDense` – this calls either `DGETRF` or `SGETRF` to perform the LU factorization.
- `SUNLinSolSolve_LapackDense` – this calls either `DGETRS` or `SGETRS` to use the LU factors and `pivots` array to perform the solve.
- `SUNLinSolLastFlag_LapackDense`
- `SUNLinSolSpace_LapackDense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- `SUNLinSolFree_LapackDense`

8.7.3 SUNLinearSolver_LapackDense Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKDENSE module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNLAPACKDENSEINIT

Call	<code>FSUNLAPACKDENSEINIT(code, ier)</code>
Description	The function <code>FSUNLAPACKDENSEINIT</code> can be called for Fortran programs to create a LAPACK-based dense <code>SUNLinearSolver</code> object.
Arguments	<code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for <code>CVODE</code> , 2 for <code>IDA</code> , 3 for <code>KINSOL</code> , and 4 for <code>ARKODE</code>).
Return value	<code>ier</code> 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 <i>after</i> both the <code>NVECTOR</code> and <code>SUNMATRIX</code> 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	<code>FSUNMASSLAPACKDENSEINIT(ier)</code>
Description	The function <code>FSUNMASSLAPACKDENSEINIT</code> can be called for Fortran programs to create a LAPACK-based, dense <code>SUNLinearSolver</code> object for mass matrix linear systems.
Arguments	None
Return value	<code>ier</code> is a <code>int</code> 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 <i>after</i> both the <code>NVECTOR</code> and <code>SUNMATRIX</code> mass-matrix objects have been initialized.

8.7.4 SUNLinearSolver_LapackDense content

The `SUNLINSOL_LAPACKDENSE` module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_Dense {
    sunindextype N;
    sunindextype *pivots;
    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.

8.8 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`.



8.8.1 SUNLinearSolver_LapackBand description

This solver is constructed to perform the following operations:

- The “setup” call performs a LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1’s on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input `SUNMATRIX_BAND` object A , with pivoting information encoding P stored in the `pivots` array.
- The “solve” call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the `SUNMATRIX_BAND` object.
- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `m1`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1, mu+m1)`. The lower triangular factor L has lower bandwidth `m1`.



8.8.2 SUNLinearSolver_LapackBand functions

The SUNLINSOL_LAPACKBAND module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

SUNLinSol_LapackBand

Call	<code>LS = SUNLinSol_LapackBand(y, A);</code>
Description	The function <code>SUNLinSol_LapackBand</code> creates and allocates memory for a LAPACK-based, band <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>A</code> (<code>SUNMatrix</code>) a <code>SUNMATRIX_BAND</code> matrix template for cloning matrices needed within the solver
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_BAND</code> matrix type and the <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> , and <code>NVECTOR_PTHREADS</code> 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 <code>A</code> is allocated with appropriate upper bandwidth storage for the LU factorization.
Deprecated Name	For backward compatibility, the wrapper function <code>SUNLapackBand</code> with identical input and output arguments is also provided.

The SUNLINSOL_LAPACKBAND module defines band implementations of all “direct” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- SUNLinSolGetType_LapackBand
- SUNLinSolInitialize_LapackBand – this does nothing, since all consistency checks are performed at solver creation.
- SUNLinSolSetup_LapackBand – this calls either DGBTRF or SGBTRF to perform the *LU* factorization.
- SUNLinSolSolve_LapackBand – this calls either DGBTRS or SGBTRS to use the *LU* factors and pivots array to perform the solve.
- SUNLinSolLastFlag_LapackBand
- SUNLinSolSpace_LapackBand – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.
- SUNLinSolFree_LapackBand

8.8.3 SUNLinearSolver_LapackBand Fortran interfaces

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_LAPACKBAND module also includes a Fortran-callable function for creating a SUNLinearSolver object.

FSUNLAPACKDENSEINIT

Call FSUNLAPACKBANDINIT(`code`, `ier`)

Description The function FSUNLAPACKBANDINIT can be called for Fortran programs to create a LAPACK-based band SUNLinearSolver object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

Return value `ier` is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX objects have been initialized.

Additionally, when using ARKODE with a non-identity mass matrix, the SUNLINSOL_LAPACKBAND module includes a Fortran-callable function for creating a SUNLinearSolver mass matrix solver object.

FSUNMASSLAPACKBANDINIT

Call FSUNMASSLAPACKBANDINIT(`ier`)

Description The function FSUNMASSLAPACKBANDINIT can be called for Fortran programs to create a LAPACK-based, band SUNLinearSolver object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the NVECTOR and SUNMATRIX mass-matrix objects have been initialized.

8.8.4 SUNLinearSolver_LapackBand content

The SUNLINSOL_LAPACKBAND module defines the *content* field of a SUNLinearSolver as the following structure:

```
struct _SUNLinearSolverContent_Band {
    sunindextype N;
    sunindextype *pivots;
    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.

8.9 The SUNLinearSolver_KLU implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with KLU. The SUNLINSOL_KLU module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

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

The SUNLINSOL_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 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 `realttype` set to either `extended` or `single` (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available `sunindextype` options.



8.9.1 SUNLinearSolver_KLU description

The KLU library has a symbolic factorization routine that computes the permutation of the linear system matrix to block triangular form and the permutations that will pre-order the diagonal blocks (the only ones that need to be factored) to reduce fill-in (using AMD, COLAMD, CHOLAMD, natural, or an ordering given by the user). Of these ordering choices, the default value in the SUNLINSOL_KLU module is the COLAMD ordering.

KLU breaks the factorization into two separate parts. The first is a symbolic factorization and the second is a numeric factorization that returns the factored matrix along with final pivot information. KLU also has a refactor routine that can be called instead of the numeric factorization. This routine will reuse the pivot information. This routine also returns diagnostic information that a user can examine to determine if numerical stability is being lost and a full numerical factorization should be done instead of the refactor.

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

- The first time that the “setup” routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.

- On subsequent calls to the “setup” routine, it calls the appropriate KLU “refactor” routine, followed by estimates of the numerical conditioning using the relevant “rcond”, and if necessary “condst”, routine(s). If these estimates of the condition number are larger than $\varepsilon^{-2/3}$ (where ε is the double-precision unit roundoff), then a new factorization is performed.
- The module includes the routine `SUNKLUReInit`, that can be called by the user to force a full or partial refactorization at the next “setup” call.
- The “solve” call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.9.2 SUNLinearSolver_KLU functions

The `SUNLINSOL_KLU` module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

<code>SUNLinSol_KLU</code>	
Call	<code>LS = SUNLinSol_KLU(y, A);</code>
Description	The function <code>SUNLinSol_KLU</code> creates and allocates memory for a KLU-based <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>A</code> (<code>SUNMatrix</code>) a <code>SUNMATRIX_SPARSE</code> matrix template for cloning matrices needed within the solver
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_SPARSE</code> matrix type (using either <code>CSR</code> or <code>CSC</code> storage formats) and the <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> , and <code>NVECTOR_PTHREADS</code> vector types. As additional compatible matrix and vector implementations are added to <code>SUNDIALS</code> , these will be included within this compatibility check.
Deprecated Name	For backward compatibility, the wrapper function <code>SUNKLU</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_KLU</code>

The `SUNLINSOL_KLU` module defines implementations of all “direct” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_KLU`
- `SUNLinSolInitialize_KLU` – this sets the `first_factorize` flag to 1, forcing both symbolic and numerical factorizations on the subsequent “setup” call.
- `SUNLinSolSetup_KLU` – this performs either a *LU* factorization or refactorization of the input matrix.
- `SUNLinSolSolve_KLU` – this calls the appropriate KLU solve routine to utilize the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_KLU`
- `SUNLinSolSpace_KLU` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the KLU documentation.

- SUNLinSolFree_KLU

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The SUNLINSOL_KLU module also defines the following additional user-callable functions.

SUNLinSol_KLUReInit	
Call	<code>retval = SUNLinSol_KLUReInit(LS, A, nnz, reinit_type);</code>
Description	The function <code>SUNLinSol_KLUReInit</code> 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 nonzeros has changed or if the structure of the linear system has changed which would require a new symbolic (and numeric factorization).
Arguments	<p><code>LS</code> (SUNLinearSolver) a template for cloning vectors needed within the solver</p> <p><code>A</code> (SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver</p> <p><code>nnz</code> (sunindextype) the new number of nonzeros in the matrix</p> <p><code>reinit_type</code> (int) flag governing the level of reinitialization. The allowed values are:</p> <ul style="list-style-type: none"> • <code>SUNKLU_REINIT_FULL</code> – The Jacobian matrix will be destroyed and a new one will be allocated based on the <code>nnz</code> value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup. • <code>SUNKLU_REINIT_PARTIAL</code> – Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of <code>nnz</code> given in the sparse matrix provided to the original constructor routine (or the previous <code>SUNLinSol_KLUReInit</code> call).
Return value	The return values from this function are <code>SUNLS_MEM_NULL</code> (either <code>S</code> or <code>A</code> are <code>NULL</code>), <code>SUNLS_ILL_INPUT</code> (<code>A</code> does not have type <code>SUNMATRIX_SPARSE</code> or <code>reinit_type</code> is invalid), <code>SUNLS_MEM_FAIL</code> (reallocation of the sparse matrix failed) or <code>SUNLS_SUCCESS</code> .
Notes	<p>This routine will perform consistency checks to ensure that it is called with consistent <code>NVECTOR</code> and <code>SUNMATRIX</code> implementations. These are currently limited to the <code>SUNMATRIX_SPARSE</code> matrix type (using either <code>CSR</code> or <code>CSC</code> storage formats) and the <code>NVECTOR_SERIAL</code>, <code>NVECTOR_OPENMP</code>, and <code>NVECTOR_PTHREADS</code> vector types. As additional compatible matrix and vector implementations are added to <code>SUNDIALS</code>, these will be included within this compatibility check.</p> <p>This routine assumes no other changes to solver use are necessary.</p>
Deprecated Name	For backward compatibility, the wrapper function <code>SUNKLUReInit</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_KLUReInit</code>

SUNLinSol_KLUSetOrdering	
Call	<code>retval = SUNLinSol_KLUSetOrdering(LS, ordering);</code>
Description	This function sets the ordering used by KLU for reducing fill in the linear solve.
Arguments	<p><code>LS</code> (SUNLinearSolver) the SUNLINSOL_KLU object</p> <p><code>ordering</code> (int) flag indicating the reordering algorithm to use, the options are:</p> <p>0 AMD,</p>

- 1 COLAMD, and
- 2 the natural ordering.

The default is 1 for COLAMD.

Return value	The return values from this function are <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>), <code>SUNLS_ILL_INPUT</code> (invalid ordering choice), or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNKLUSetOrdering</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_KLUSetOrdering</code>

`SUNLinSol_KLUGetSymbolic`

Call	<code>symbolic = SUNLinSol_KLUGetSymbolic(LS);</code>
Description	This function returns a pointer to the KLU symbolic factorization stored in the <code>SUNLINSOL_KLU content</code> structure.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_KLU</code> object
Return value	The return type from this function is <code>sun_klu_symbolic</code> .
Notes	When <code>SUNDIALS</code> is compiled with 32-bit indices (<code>SUNDIALS_INDEX_SIZE=32</code>), <code>sun_klu_symbolic</code> is mapped to the KLU type <code>klu_symbolic</code> ; when <code>SUNDIALS</code> is compiled with 64-bit indices (<code>SUNDIALS_INDEX_SIZE=64</code>) this is mapped to the KLU type <code>klu_l_symbolic</code> .

`SUNLinSol_KLUGetNumeric`

Call	<code>numeric = SUNLinSol_KLUGetNumeric(LS);</code>
Description	This function returns a pointer to the KLU numeric factorization stored in the <code>SUNLINSOL_KLU content</code> structure.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_KLU</code> object
Return value	The return type from this function is <code>sun_klu_numeric</code> .
Notes	When <code>SUNDIALS</code> is compiled with 32-bit indices (<code>SUNDIALS_INDEX_SIZE=32</code>), <code>sun_klu_numeric</code> is mapped to the KLU type <code>klu_numeric</code> ; when <code>SUNDIALS</code> is compiled with 64-bit indices (<code>SUNDIALS_INDEX_SIZE=64</code>), this is mapped to the KLU type <code>klu_l_numeric</code> .

`SUNLinSol_KLUGetCommon`

Call	<code>common = SUNLinSol_KLUGetCommon(LS);</code>
Description	This function returns a pointer to the KLU common structure stored within in the <code>SUNLINSOL_KLU content</code> structure.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_KLU</code> object
Return value	The return type from this function is <code>sun_klu_common</code> .
Notes	When <code>SUNDIALS</code> is compiled with 32-bit indices (<code>SUNDIALS_INDEX_SIZE=32</code>), <code>sun_klu_common</code> is mapped to the KLU type <code>klu_common</code> ; when <code>SUNDIALS</code> is compiled with 64-bit indices (<code>SUNDIALS_INDEX_SIZE=64</code>), this is mapped to the KLU type <code>klu_l_common</code> .

8.9.3 `SUNLinearSolver_KLU` Fortran interfaces

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

FORTRAN 2003 interface module

The `fsunlinsol_klu_mod` FORTRAN module defines interfaces to all SUNLINSOL_KLU C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading ‘F’. For example, the function `SUNLinSol_klu` is interfaced as `FSUNLinSol_klu`.

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

FORTRAN 77 interface functions

For solvers that include a FORTRAN 77 interface module, the SUNLINSOL_KLU module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNKLUINIT

Call `FSUNKLUINIT(code, ier)`

Description The function `FSUNKLUINIT` can be called for Fortran programs to create a `SUNLINSOL_KLU` object.

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for `CVODE`, 2 for `IDA`, 3 for `KINSOL`, and 4 for `ARKODE`).

Return value `ier` is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the `NVECTOR` and `SUNMATRIX` objects have been initialized.

Additionally, when using `ARKODE` with a non-identity mass matrix, the `SUNLINSOL_KLU` module includes a Fortran-callable function for creating a `SUNLinearSolver` mass matrix solver object.

FSUNMASSKLUINIT

Call `FSUNMASSKLUINIT(ier)`

Description The function `FSUNMASSKLUINIT` can be called for Fortran programs to create a KLU-based `SUNLinearSolver` object for mass matrix linear systems.

Arguments None

Return value `ier` is a `int` return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes This routine must be called *after* both the `NVECTOR` and `SUNMATRIX` mass-matrix objects have been initialized.

The `SUNLinSol_KLUReInit` and `SUNLinSol_KLUSetOrdering` routines also support FORTRAN interfaces for the system and mass matrix solvers:

FSUNKLUREINIT

Call `FSUNKLUREINIT(code, nnz, reinit_type, ier)`

Description The function `FSUNKLUREINIT` can be called for Fortran programs to re-initialize a `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.

8.9.4 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).

8.10 The SUNLinearSolver_SuperLUDIST implementation

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

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

8.10.1 SUNLinearSolver_SuperLUDIST description

The SUNLINSOL_SUPERLUDIST module is a SUNLINSOL adapter for the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li [3, 23, 37, 38]. 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 `DGFACT` so that a subsequent call to the “solve” routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to solve the system.
- On subsequent calls to the “setup” routine, it sets the SuperLU_DIST option `Fact` to `SamePattern` so that a subsequent call to “solve” will perform factorization assuming the same sparsity pattern as prior, i.e. it will reuse the column permutation vector.
- If “setup” is called prior to the “solve” routine, then the “solve” routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to the sparse triangular solves, and, potentially, iterative refinement. If “setup” is not called prior, “solve” will skip to the triangular solve step. We note that in this solve SuperLU_DIST operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.10.2 SUNLinearSolver_SuperLUDIST functions

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

- `SUNLinSolGetType_SuperLUDIST`
- `SUNLinSolInitialize_SuperLUDIST` – this sets the `first_factorize` flag to 1 and resets the internal SuperLU_DIST statistics variables.
- `SUNLinSolSetup_SuperLUDIST` – this sets the appropriate SuperLU_DIST options so that a subsequent solve will perform a symbolic and numerical factorization before proceeding with the triangular solves
- `SUNLinSolSolve_SuperLUDIST` – this calls the SuperLU_DIST solve routine to perform factorization (if the setup routine was called prior) and then use the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_SuperLUDIST`
- `SUNLinSolSpace_SuperLUDIST` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SuperLU_DIST documentation.
- `SUNLinSolFree_SuperLUDIST`

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

SUNLinSol_SuperLUDIST

Call `LS = SUNLinSol_SuperLUDIST(y, A, grid, lu, scaleperm, solve, stat, options);`

Description The function `SUNLinSol_SuperLUDIST` creates and allocates memory for a `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

8.10.3 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;
  reatype         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

8.11 The SUNLinearSolver_SuperLUMT implementation

This section describes the SUNLINSOL implementation for solving sparse linear systems with SuperLU_MT. The SUPERLUMT module is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory NVECTOR implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). While these are compatible, it is not recommended to use a threaded vector module with SUNLINSOL_SUPERLUMT unless it is the NVECTOR_OPENMP module and the SUPERLUMT library has also been compiled with OpenMP.

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

The SUNLINSOL_SUPERLUMT module is a SUNLINSOL wrapper for the SUPERLUMT sparse matrix factorization and solver library written by X. Sherry Li [4, 36, 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.



8.11.1 SUNLinearSolver_SuperLUMT description

The SUPERLUMT library has a symbolic factorization routine that computes the permutation of the linear system matrix to reduce fill-in on subsequent LU factorizations (using COLAMD, minimal degree ordering on $A^T * A$, minimal degree ordering on $A^T + A$, or natural ordering). Of these ordering choices, the default value in the SUNLINSOL_SUPERLUMT module is the COLAMD ordering.

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

- The first time that the “setup” routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.
- On subsequent calls to the “setup” routine, it skips the symbolic factorization, and only refactors the input matrix.
- The “solve” call performs pivoting and forward and backward substitution using the stored SUPERLUMT data structures. We note that in this solve SUPERLUMT operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

8.11.2 SUNLinearSolver_SuperLUMT functions

The module SUNLINSOL_SUPERLUMT provides the following user-callable constructor for creating a `SUNLinearSolver` object.

<code>SUNLinSol_SuperLUMT</code>	
Call	<code>LS = SUNLinSol_SuperLUMT(y, A, num_threads);</code>
Description	The function <code>SUNLinSol_SuperLUMT</code> creates and allocates memory for a SuperLU_MT-based <code>SUNLinearSolver</code> object.
Arguments	<p><code>y</code> (N_Vector) a template for cloning vectors needed within the solver</p> <p><code>A</code> (SUNMatrix) a SUNMATRIX_SPARSE matrix template for cloning matrices needed within the solver</p> <p><code>num_threads</code> (int) desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps</p>
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>A</code> or <code>y</code> are incompatible then this routine will return <code>NULL</code> .
Notes	<p>This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SUPERLUMT library.</p> <p>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.</p> <p>The <code>num_threads</code> argument is not checked and is passed directly to SUPERLUMT routines.</p>

Deprecated Name For backward compatibility, the wrapper function `SUNSuperLUMT` with identical input and output arguments is also provided.

The `SUNLINSOL_SUPERLUMT` module defines implementations of all “direct” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_SuperLUMT`
- `SUNLinSolInitialize_SuperLUMT` – this sets the `first_factorize` flag to 1 and resets the internal SUPERLUMT statistics variables.
- `SUNLinSolSetup_SuperLUMT` – this performs either a *LU* factorization or refactorization of the input matrix.
- `SUNLinSolSolve_SuperLUMT` – this calls the appropriate SUPERLUMT solve routine to utilize the *LU* factors to solve the linear system.
- `SUNLinSolLastFlag_SuperLUMT`
- `SUNLinSolSpace_SuperLUMT` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SUPERLUMT documentation.
- `SUNLinSolFree_SuperLUMT`

The `SUNLINSOL_SUPERLUMT` module also defines the following additional user-callable function.

SUNLinSol_SuperLUMTSetOrdering

Call	<code>retval = SUNLinSol_SuperLUMTSetOrdering(LS, ordering);</code>
Description	This function sets the ordering used by SUPERLUMT for reducing fill in the linear solve.
Arguments	<p><code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SUPERLUMT</code> object</p> <p><code>ordering</code> (<code>int</code>) a flag indicating the ordering algorithm to use, the options are:</p> <ul style="list-style-type: none"> 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 <p>The default is 3 for COLAMD.</p>
Return value	The return values from this function are <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>), <code>SUNLS_ILL_INPUT</code> (invalid ordering choice), or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSuperLUMTSetOrdering</code> with identical input and output arguments is also provided.

8.11.3 SUNLinearSolver_SuperLUMT Fortran interfaces

For solvers that include a Fortran interface module, the `SUNLINSOL_SUPERLUMT` module also includes a Fortran-callable function for creating a `SUNLinearSolver` object.

FSUNSUPERLUMTINIT

Call	<code>FSUNSUPERLUMTINIT(code, num_threads, ier)</code>
Description	The function <code>FSUNSUPERLUMTINIT</code> can be called for Fortran programs to create a <code>SUNLINSOL_KLU</code> object.
Arguments	<p><code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for <code>CVODE</code>, 2 for <code>IDA</code>, 3 for <code>KINSOL</code>, and 4 for <code>ARKODE</code>).</p>

`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.

8.11.4 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.

8.12 The SUNLinearSolver_cuSolverSp_batchQR implementation

The `SUNLinearSolver_cuSolverSp_batchQR` implementation of the `SUNLINSOL` API is designed to be used with the `SUNMATRIX_CUSPARSE` matrix, and the `NVECTOR_CUDA` vector. The header file to include when using this module is `sunlinsol/sunlinsol_cusolversp_batchqr.h`. The installed library to link to is `libsundials_sunlinsolcusolversp.lib` where *.lib* is typically *.so* for shared libraries and *.a* for static libraries.

The `SUNLinearSolver_cuSolverSp_batchQR` module is experimental and subject to change.



8.12.1 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

$$\begin{bmatrix} \mathbf{A}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{A}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A}_n \end{bmatrix} x_j = b_j$$

where all block matrices \mathbf{A}_j share the same sparsity pattern. The matrix must be the `SUNMATRIX_CUSPAESE` module.

8.12.2 SUNLinearSolver_cuSolverSp_batchQR functions

The `SUNLinearSolver_cuSolverSp_batchQR` module defines implementations of all “direct” linear solver operations listed in Sections 8.1.1-8.1.3:

- `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, csol);`

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
`csol` (`cusolverHandle_t`) a valid cuSOLVER handle

Return value This returns a `SUNLinearSolver` object. If either `A` or `y` are incompatible then this routine will return `NULL`.

Notes This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the solver.

This routine will perform consistency checks to ensure that it is called with consistent `NVECTOR` and `SUNMATRIX` implementations. These are currently limited to the `SUNMAT_CUSPARSE` matrix type and the `NVECTOR_CUDA` vector type. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

SUNLinSol_cuSolverSp_batchQR_GetDescription

Call `SUNLinSol_cuSolverSp_batchQR_GetDescription(LS, &desc);`

Description The function `SUNLinSol_cuSolverSp_batchQR_GetDescription` accesses the string description of the object (empty by default).

Arguments `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
`desc` (`char **`) the string description of the linear solver

Return value None

SUNLinSol_cuSolverSp_batchQR_SetDescription

Call `SUNLinSol_cuSolverSp_batchQR_SetDescription(LS, desc);`

Description The function `SUNLinSol_cuSolverSp_batchQR_SetDescription` sets the string description of the object (empty by default).

Arguments `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
`desc` (`const char *`) the string description of the linear solver

Return value None

SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace

Call `SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace(LS, cuSolverInternal, cuSolverWorkspace);`

Description The function `SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace` returns the `cuSOLVER` batch QR method internal buffer size, in bytes, in the argument `cuSolverInternal` and the `cuSOLVER` batch QR workspace buffer size, in bytes, in the argument `cuSolverWorkspace`. The size of the internal buffer is proportional to the number of matrix blocks while the size of the workspace is almost independent of the number of blocks.

Arguments `LS` (`SUNLinearSolver`) a `SUNLinSol_cuSolverSp_batchQR` object
`cuSolverInternal` (`size_t *`) output – the size of the `cuSOLVER` internal buffer in bytes
`cuSolverWorkspace` (`size_t *`) output – the size of the `cuSOLVER` workspace buffer in bytes

Return value None

8.12.3 SUNLinearSolver_cuSolverSp_batchQR content

The `SUNLinearSolver_cuSolverSp_batchQR` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_cuSolverSp_batchQR {
    int                last_flag;           /* last return flag */
    booleantype       first_factorize;     /* is this the first factorization? */
    size_t            internal_size;       /* size of cusolver internal buffer for Q and R */
    size_t            workspace_size;     /* size of cusolver memory block for num. factorization */
    cusolverSpHandle_t  cusolver_handle;   /* cuSolverSp context */
    csrqrInfo_t       info;               /* opaque cusolver data structure */
    void*             workspace;          /* memory block used by cusolver */
    const char*       desc;               /* description of this linear solver */
};
```

8.13 The SUNLinearSolver_SPGMR implementation

This section describes the SUNLINSOL implementation of the SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [43]) iterative linear solver. The SUNLINSOL_SPGMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (N_VClone, N_VDotProd, N_VScale, N_VLinearSum, N_VProd, N_VConst, N_VDiv, and N_VDestroy). When using Classical Gram-Schmidt, the optional function N_VDotProdMulti may be supplied for increased efficiency.

To access the SUNLINSOL_SPGMR module, include the header file `sunlinsol/sunlinsol_spgmr.h`. We note that the SUNLINSOL_SPGMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspgmr` module library.

8.13.1 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.

8.13.2 SUNLinearSolver_SPGMR functions

The SUNLINSOL_SPGMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

<code>SUNLinSol_SPGMR</code>	
Call	<code>LS = SUNLinSol_SPGMR(y, pretype, max1);</code>
Description	The function <code>SUNLinSol_SPGMR</code> creates and allocates memory for a SPGMR <code>SUNLinearSolver</code> object.
Arguments	<p><code>y</code> (N_Vector) a template for cloning vectors needed within the solver</p> <p><code>pretype</code> (int) flag indicating the desired type of preconditioning, allowed values are:</p> <ul style="list-style-type: none"> • <code>PREC_NONE</code> (0) • <code>PREC_LEFT</code> (1) • <code>PREC_RIGHT</code> (2) • <code>PREC_BOTH</code> (3) <p>Any other integer input will result in the default (no preconditioning).</p> <p><code>max1</code> (int) the number of Krylov basis vectors to use. Values ≤ 0 will result in the default value (5).</p>
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>y</code> is incompatible then this routine will return <code>NULL</code> .

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 identical 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 8.1.1 – 8.1.3:

- `SUNLinSolGetType_SPGMR`
- `SUNLinSolInitialize_SPGMR`
- `SUNLinSolSetATimes_SPGMR`
- `SUNLinSolSetPreconditioner_SPGMR`
- `SUNLinSolSetScalingVectors_SPGMR`
- `SUNLinSolSetup_SPGMR`
- `SUNLinSolSolve_SPGMR`
- `SUNLinSolNumIters_SPGMR`
- `SUNLinSolResNorm_SPGMR`
- `SUNLinSolResid_SPGMR`
- `SUNLinSolLastFlag_SPGMR`
- `SUNLinSolSpace_SPGMR`
- `SUNLinSolFree_SPGMR`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The `SUNLINSOL_SPGMR` module also defines the following additional user-callable functions.

`SUNLinSol_SPGMRSetPrecType`

Call `retval = SUNLinSol_SPGMRSetPrecType(LS, pretype);`

Description The function `SUNLinSol_SPGMRSetPrecType` updates the type of preconditioning to use in the `SUNLINSOL_SPGMR` object.

Arguments `LS` (`SUNLinearSolver`) the `SUNLINSOL_SPGMR` object to update
`pretype` (`int`) flag indicating the desired type of preconditioning, allowed values match those discussed in `SUNLinSol_SPGMR`.

Return value This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

Deprecated Name For backward compatibility, the wrapper function `SUNSPGMRSetPrecType` with identical input and output arguments is also provided.

F2003 Name `FSUNLinSol_SPGMRSetPrecType`

SUNLinSol_SPGMRSetGSType

Call	<code>retval = SUNLinSol_SPGMRSetGSType(LS, gstype);</code>
Description	The function <code>SUNLinSol_SPGMRSetPrecType</code> sets the type of Gram-Schmidt orthogonalization to use in the <code>SUNLINSOL_SPGMR</code> object.
Arguments	<p><code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPGMR</code> object to update</p> <p><code>gstype</code> (<code>int</code>) flag indicating the desired orthogonalization algorithm; allowed values are:</p> <ul style="list-style-type: none"> • <code>MODIFIED_GS</code> (1) • <code>CLASSICAL_GS</code> (2) <p>Any other integer input will result in a failure, returning error code <code>SUNLS_ILL_INPUT</code>.</p>
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPGMRSetGSType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPGMRSetGSType</code>

SUNLinSol_SPGMRSetMaxRestarts

Call	<code>retval = SUNLinSol_SPGMRSetMaxRestarts(LS, maxrs);</code>
Description	The function <code>SUNLinSol_SPGMRSetMaxRestarts</code> sets the number of GMRES restarts to allow in the <code>SUNLINSOL_SPGMR</code> object.
Arguments	<p><code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPGMR</code> object to update</p> <p><code>maxrs</code> (<code>int</code>) integer indicating number of restarts to allow. A negative input will result in the default of 0.</p>
Return value	This routine will return with one of the error codes <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPGMRSetMaxRestarts</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPGMRSetMaxRestarts</code>

8.13.3 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_fsunlinsol_spgmr_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_fsunlinsol_spgmr_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 orthogonalization 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 orthogonalization 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>code</code> is not needed since mass matrix linear systems only arise in ARKODE.
Return value	<code>ier</code> is a <code>int</code> 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.

8.13.4 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:

<code>maxl</code>	- number of GMRES basis vectors to use (default is 5),
<code>pretype</code>	- flag for type of preconditioning to employ (default is none),
<code>gstype</code>	- flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),
<code>max_restarts</code>	- number of GMRES restarts to allow (default is 0),
<code>numiters</code>	- number of iterations from the most-recent solve,
<code>resnorm</code>	- final linear residual norm from the most-recent solve,
<code>last_flag</code>	- last error return flag from an internal function,
<code>ATimes</code>	- function pointer to perform Av product,
<code>ATData</code>	- pointer to structure for <code>ATimes</code> ,
<code>Psetup</code>	- function pointer to preconditioner setup routine,

- In the “initialize” call, the remaining solver data is allocated (`v`, `Hes`, `givens`, and `yg`)
- In the “setup” call, any non-NULL `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).
- In the “solve” call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

8.14.2 SUNLinearSolver_SPFGMR functions

The `SUNLINSOL_SPFGMR` module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

<code>SUNLinSol_SPFGMR</code>	
Call	<code>LS = SUNLinSol_SPFGMR(y, pretype, maxl);</code>
Description	The function <code>SUNLinSol_SPFGMR</code> creates and allocates memory for a <code>SPFGMR SUNLinearSolver</code> object.
Arguments	<p><code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver</p> <p><code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values are:</p> <ul style="list-style-type: none"> • <code>PREC_NONE</code> (0) • <code>PREC_LEFT</code> (1) • <code>PREC_RIGHT</code> (2) • <code>PREC_BOTH</code> (3) <p>Any other integer input will result in the default (no preconditioning).</p> <p><code>maxl</code> (<code>int</code>) the number of Krylov basis vectors to use. Values ≤ 0 will result in the default value (5).</p>
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>y</code> is incompatible then this routine will return <code>NULL</code> .
Notes	<p>This routine will perform consistency checks to ensure that it is called with a consistent <code>NVECTOR</code> implementation (i.e. that it supplies the requisite vector operations). If <code>y</code> is incompatible, then this routine will return <code>NULL</code>.</p> <p>We note that some SUNDIALS solvers are designed to only work with left preconditioning (<code>IDA</code> and <code>IDAS</code>) and others with only right preconditioning (<code>KINSOL</code>). While it is possible to configure a <code>SUNLINSOL_SPFGMR</code> object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.</p>

F2003 Name `FSUNLinSol_SPFGMR`

SUNSPFGMR The `SUNLINSOL_SPFGMR` module defines implementations of all “iterative” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_SPFGMR`
- `SUNLinSolInitialize_SPFGMR`
- `SUNLinSolSetATimes_SPFGMR`
- `SUNLinSolSetPreconditioner_SPFGMR`
- `SUNLinSolSetScalingVectors_SPFGMR`
- `SUNLinSolSetup_SPFGMR`
- `SUNLinSolSolve_SPFGMR`

- SUNLinSolNumIters_SPFGMR
- SUNLinSolResNorm_SPFGMR
- SUNLinSolResid_SPFGMR
- SUNLinSolLastFlag_SPFGMR
- SUNLinSolSpace_SPFGMR
- SUNLinSolFree_SPFGMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The SUNLINSOL_SPFGMR module also defines the following additional user-callable functions.

SUNLinSol_SPFGMRSetPrecType

Call	<code>retval = SUNLinSol_SPFGMRSetPrecType(LS, pretype);</code>
Description	The function <code>SUNLinSol_SPFGMRSetPrecType</code> updates the type of preconditioning to use in the <code>SUNLINSOL_SPFGMR</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPFGMR</code> object to update <code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values match those discussed in <code>SUNLinSol_SPFGMR</code> .
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPFGMRSetPrecType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPFGMRSetPrecType</code>

SUNLinSol_SPFGMRSetGSType

Call	<code>retval = SUNLinSol_SPFGMRSetGSType(LS, gstype);</code>
Description	The function <code>SUNLinSol_SPFGMRSetGSType</code> sets the type of Gram-Schmidt orthogonalization to use in the <code>SUNLINSOL_SPFGMR</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPFGMR</code> object to update <code>gstype</code> (<code>int</code>) flag indicating the desired orthogonalization algorithm; allowed values are: <ul style="list-style-type: none"> • <code>MODIFIED_GS</code> (1) • <code>CLASSICAL_GS</code> (2) Any other integer input will result in a failure, returning error code <code>SUNLS_ILL_INPUT</code> .
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPFGMRSetGSType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPFGMRSetGSType</code>

SUNLinSol_SPFGMRSetMaxRestarts

Call	<code>retval = SUNLinSol_SPFGMRSetMaxRestarts(LS, maxrs);</code>
Description	The function <code>SUNLinSol_SPFGMRSetMaxRestarts</code> sets the number of GMRES restarts to allow in the <code>SUNLINSOL_SPFGMR</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPFGMR</code> object to update <code>maxrs</code> (<code>int</code>) 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 <code>SUNLS_MEM_NULL</code> (S is NULL) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPFGMRSetMaxRestarts</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPFGMRSetMaxRestarts</code>

8.14.3 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.

FORTTRAN 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.

FORTTRAN 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	<code>FSUNSPFGMRINIT(code, pretype, maxl, ier)</code>
Description	The function <code>FSUNSPFGMRINIT</code> can be called for Fortran programs to create a <code>SUNLINSOL_SPFGMR</code> object.
Arguments	<code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for <code>CVODE</code> , 2 for <code>IDA</code> , 3 for <code>KINSOL</code> , and 4 for <code>ARKODE</code>). <code>pretype</code> (<code>int*</code>) flag indicating desired preconditioning type <code>maxl</code> (<code>int*</code>) flag indicating Krylov subspace size
Return value	<code>ier</code> 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 <i>after</i> the <code>NVECTOR</code> object has been initialized. Allowable values for <code>pretype</code> and <code>maxl</code> are the same as for the C function <code>SUNLinSol_SPFGMR</code> .

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.

FSUNMASSSPFGMRINIT

Call FSUNMASSSPFGMRINIT(*pretype*, *maxl*, *ier*)

Description The function FSUNMASSSPFGMRINIT 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.

FSUNSPFGMRSETGSTYPE

Call FSUNSPFGMRSETGSTYPE(*code*, *gstype*, *ier*)

Description The function FSUNSPFGMRSETGSTYPE can be called for Fortran programs to change the Gram-Schmidt orthogonalization 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.

FSUNMASSSPFGMRSETGSTYPE

Call FSUNMASSSPFGMRSETGSTYPE(*gstype*, *ier*)

Description The function FSUNMASSSPFGMRSETGSTYPE can be called for Fortran programs to change the Gram-Schmidt orthogonalization 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_SPGMRSetGStype 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(prettype, 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.

8.14.4 SUNLinearSolver_SPFGMR content

The `SUNLINSOL_SPFGMR` module defines the *content* field of a `SUNLinearSolver` as the following structure:

```
struct _SUNLinearSolverContent_SPFGMR {
    int maxl;
    int prettype;
    int gstype;
    int max_restarts;
    int numiters;
```


are represented in the `givens` vector as `givens[0] = c0`, `givens[1] = s0`, `givens[2] = c1`, `givens[3] = s1`, ... `givens[2j] = cj`, `givens[2j+1] = sj`.

`xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

`yg` - a length `(maxl+1)` array of `realttype` values used to hold “short” vectors (e.g. `y` and `g`),

`vtemp` - temporary vector storage.

8.15 The SUNLinearSolver_SPBCGS implementation

This section describes the SUNLINSOL implementation of the SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [44]) iterative linear solver. The SUNLINSOL_SPBCGS module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VDiv`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, SPBCGS requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_SPBCGS module, include the header file `sunlinsol/sunlinsol_spbcgs.h`. We note that the SUNLINSOL_SPBCGS module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolspbcgs` module library.

8.15.1 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.

8.15.2 SUNLinearSolver_SPBCGS functions

The SUNLINSOL_SPBCGS module provides the following user-callable constructor for creating a `SUNLinearSolver` object.

<code>SUNLinSol_SPBCGS</code>	
Call	<code>LS = SUNLinSol_SPBCGS(y, pretype, maxl);</code>
Description	The function <code>SUNLinSol_SPBCGS</code> creates and allocates memory for a SPBCGS <code>SUNLinearSolver</code> object.
Arguments	<code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver <code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values are: <ul style="list-style-type: none"> • <code>PREC_NONE</code> (0)

- PREC_LEFT (1)
- PREC_RIGHT (2)
- PREC_BOTH (3)

Any other integer input will result in the default (no preconditioning).

`max1` (`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 identical 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 8.1.1 – 8.1.3:

- `SUNLinSolGetType_SPBCGS`
- `SUNLinSolInitialize_SPBCGS`
- `SUNLinSolSetATimes_SPBCGS`
- `SUNLinSolSetPreconditioner_SPBCGS`
- `SUNLinSolSetScalingVectors_SPBCGS`
- `SUNLinSolSetup_SPBCGS`
- `SUNLinSolSolve_SPBCGS`
- `SUNLinSolNumIters_SPBCGS`
- `SUNLinSolResNorm_SPBCGS`
- `SUNLinSolResid_SPBCGS`
- `SUNLinSolLastFlag_SPBCGS`
- `SUNLinSolSpace_SPBCGS`
- `SUNLinSolFree_SPBCGS`

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The `SUNLINSOL_SPBCGS` module also defines the following additional user-callable functions.

SUNLinSol_SPBCGSSetPrecType

Call	<code>retval = SUNLinSol_SPBCGSSetPrecType(LS, pretype);</code>
Description	The function <code>SUNLinSol_SPBCGSSetPrecType</code> updates the type of preconditioning to use in the <code>SUNLINSOL_SPBCGS</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPBCGS</code> object to update <code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values match those discussed in <code>SUNLinSol_SPBCGS</code> .
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPBCGSSetPrecType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPBCGSSetPrecType</code>

SUNLinSol_SPBCGSsetMax1

Call	<code>retval = SUNLinSol_SPBCGSsetMax1(LS, max1);</code>
Description	The function <code>SUNLinSol_SPBCGSsetMax1</code> updates the number of linear solver iterations to allow.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPBCGS</code> object to update <code>max1</code> (<code>int</code>) 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 <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPBCGSsetMax1</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPBCGSsetMax1</code>

8.15.3 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.

FORTTRAN 2003 interface module

The `fsunlinsol_spgbcs_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_spgbcs_mod`, and linking to the library `libsundials_fsunlinsolspgbcs_mod.lib` in addition to the C library. For details on where the library and module file `fsunlinsol_spgbcs_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_fsunlinsolspgbcs_mod` library.

FORTTRAN 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.

8.15.4 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.

8.16 The SUNLinearSolver_SPTFQMR implementation

This section describes the SUNLINSOL implementation of the SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [22]) iterative linear solver. The SUNLINSOL_SPTFQMR module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (**N_VClone**, **N_VDotProd**, **N_VScale**, **N_VLinearSum**, **N_VProd**, **N_VConst**, **N_VDiv**, and **N_VDestroy**). Unlike the SPGMR and SPFGMR algorithms, SPTFQMR requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_SPTFQMR module, include the header file `sunlinsol/sunlinsol_sptfqmr.h`. We note that the SUNLINSOL_SPTFQMR module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolsptfqmr` module library.

8.16.1 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.

8.16.2 SUNLinearSolver_SPTFQMR functions

The SUNLINSOL_SPTFQMR module provides the following user-callable constructor for creating a SUNLinearSolver object.

SUNLinSol_SPTFQMR	
Call	<code>LS = SUNLinSol_SPTFQMR(y, pretype, maxl);</code>
Description	The function <code>SUNLinSol_SPTFQMR</code> creates and allocates memory for a <code>SPTFQMR SUNLinearSolver</code> object.
Arguments	<p><code>y</code> (<code>N_Vector</code>) a template for cloning vectors needed within the solver</p> <p><code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values are:</p> <ul style="list-style-type: none"> • <code>PREC_NONE</code> (0) • <code>PREC_LEFT</code> (1) • <code>PREC_RIGHT</code> (2) • <code>PREC_BOTH</code> (3) <p>Any other integer input will result in the default (no preconditioning).</p> <p><code>maxl</code> (<code>int</code>) the number of linear iterations to allow. Values ≤ 0 will result in the default value (5).</p>
Return value	This returns a <code>SUNLinearSolver</code> object. If either <code>y</code> is incompatible then this routine will return <code>NULL</code> .
Notes	<p>This routine will perform consistency checks to ensure that it is called with a consistent <code>NVECTOR</code> implementation (i.e. that it supplies the requisite vector operations). If <code>y</code> is incompatible, then this routine will return <code>NULL</code>.</p> <p>We note that some <code>SUNDIALS</code> solvers are designed to only work with left preconditioning (<code>IDA</code> and <code>IDAS</code>) and others with only right preconditioning (<code>KINSOL</code>). While it is possible to configure a <code>SUNLINSOL_SPTFQMR</code> object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.</p>
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPTFQMR</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPTFQMR</code>

The `SUNLINSOL_SPTFQMR` module defines implementations of all “iterative” linear solver operations listed in Sections 8.1.1 – 8.1.3:

- `SUNLinSolGetType_SPTFQMR`
- `SUNLinSolInitialize_SPTFQMR`
- `SUNLinSolSetATimes_SPTFQMR`
- `SUNLinSolSetPreconditioner_SPTFQMR`
- `SUNLinSolSetScalingVectors_SPTFQMR`
- `SUNLinSolSetup_SPTFQMR`
- `SUNLinSolSolve_SPTFQMR`
- `SUNLinSolNumIters_SPTFQMR`
- `SUNLinSolResNorm_SPTFQMR`
- `SUNLinSolResid_SPTFQMR`

- SUNLinSolLastFlag_SPTFQMR
- SUNLinSolSpace_SPTFQMR
- SUNLinSolFree_SPTFQMR

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The SUNLINSOL_SPTFQMR module also defines the following additional user-callable functions.

SUNLinSol_SPTFQMRSetPrecType

Call	<code>retval = SUNLinSol_SPTFQMRSetPrecType(LS, pretype);</code>
Description	The function <code>SUNLinSol_SPTFQMRSetPrecType</code> updates the type of preconditioning to use in the <code>SUNLINSOL_SPTFQMR</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPTFQMR</code> object to update <code>pretype</code> (<code>int</code>) flag indicating the desired type of preconditioning, allowed values match those discussed in <code>SUNLinSol_SPTFQMR</code> .
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNSPTFQMRSetPrecType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_SPTFQMRSetPrecType</code>

SUNLinSol_SPTFQMRSetMax1

Call	<code>retval = SUNLinSol_SPTFQMRSetMax1(LS, max1);</code>
Description	The function <code>SUNLinSol_SPTFQMRSetMax1</code> updates the number of linear solver iterations to allow.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_SPTFQMR</code> object to update <code>max1</code> (<code>int</code>) 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 <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
F2003 Name	<code>FSUNLinSol_SPTFQMRSetMax1</code>
	<code>SUNSPTFQMRSetMax1</code>

8.16.3 SUNLinearSolver_SPTFQMR Fortran interfaces

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

FORTTRAN 2003 interface module

The `fsunlinsol_sptfqmr_mod` FORTRAN module defines interfaces to all `SUNLINSOL_SPTFQMR` 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_SPTFQMR` 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 CVOICE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).
maxl (*int**) the number of iterations to allow.

Return value *ier* is a *int* return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

FSUNMASSSPTFQMRSETMAXL

Call FSUNMASSSPTFQMRSETMAXL(*maxl*, *ier*)

Description The function FSUNMASSSPTFQMRSETMAXL can be called for Fortran programs to change the type of preconditioning for mass matrix linear systems.

Arguments The arguments are identical to FSUNSPTFQMRSETMAXL above, except that *code* is not needed since mass matrix linear systems only arise in ARKODE.

Return value *ier* is a *int* return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

Notes See SUNLinSol_SPTFQMRSetMaxl for complete further documentation of this routine.

8.16.4 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.

8.17 The SUNLinearSolver_PCG implementation

This section describes the SUNLINSOL implementation of the PCG (Preconditioned Conjugate Gradient [24]) iterative linear solver. The SUNLINSOL_PCG module is designed to be compatible with any NVECTOR implementation that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, and `N_VDestroy`). Unlike the SPGMR and SPFGMR algorithms, PCG requires a fixed amount of memory that does not increase with the number of allowed iterations.

To access the SUNLINSOL_PCG module, include the header file `sunlinsol/sunlinsol_pcg.h`. We note that the SUNLINSOL_PCG module is accessible from SUNDIALS packages *without* separately linking to the `libsundials_sunlinsolpcg` module library.

8.17.1 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

$$\tilde{A}\tilde{x} = \tilde{b} \quad (8.4)$$

where

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

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

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

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.

8.17.2 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, max1);
Description	The function SUNLinSol_PCG creates and allocates memory for a PCG SUNLinearSolver object.
Arguments	<p>y (N_Vector) a template for cloning vectors needed within the solver</p> <p>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).</p> <p>max1 (int) the number of linear iterations to allow; values ≤ 0 will result in the default value (5).</p>
Return value	This returns a SUNLinearSolver object. If either y is incompatible then this routine will return NULL.
Notes	<p>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.</p> <p>Although some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL), PCG should <i>only</i> be used with these packages when the linear systems are known to be <i>symmetric</i>. 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.</p>
Deprecated Name	For backward compatibility, the wrapper function SUNPCG with identical 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 8.1.1 – 8.1.3:

- SUNLinSolGetType_PCG
- SUNLinSolInitialize_PCG
- SUNLinSolSetATimes_PCG
- SUNLinSolSetPreconditioner_PCG
- SUNLinSolSetScalingVectors_PCG – since PCG only supports symmetric scaling, the second NVECTOR argument to this function is ignored
- SUNLinSolSetup_PCG
- SUNLinSolSolve_PCG
- SUNLinSolNumIters_PCG
- SUNLinSolResNorm_PCG
- SUNLinSolResid_PCG
- SUNLinSolLastFlag_PCG
- SUNLinSolSpace_PCG
- SUNLinSolFree_PCG

All of the listed operations are callable via the FORTRAN 2003 interface module by prepending an ‘F’ to the function name.

The SUNLINSOL_PCG module also defines the following additional user-callable functions.

SUNLinSol_PCGSetPrecType

Call	<code>retval = SUNLinSol_PCGSetPrecType(LS, pretype);</code>
Description	The function <code>SUNLinSol_PCGSetPrecType</code> updates the flag indicating use of preconditioning in the <code>SUNLINSOL_PCG</code> object.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_PCG</code> object to update <code>pretype</code> (<code>int</code>) flag indicating use of preconditioning, allowed values match those discussed in <code>SUNLinSol_PCG</code> .
Return value	This routine will return with one of the error codes <code>SUNLS_ILL_INPUT</code> (illegal <code>pretype</code>), <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNPCGSetPrecType</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_PCGSetPrecType</code>

SUNLinSol_PCGSetMax1

Call	<code>retval = SUNLinSol_PCGSetMax1(LS, max1);</code>
Description	The function <code>SUNLinSol_PCGSetMax1</code> updates the number of linear solver iterations to allow.
Arguments	<code>LS</code> (<code>SUNLinearSolver</code>) the <code>SUNLINSOL_PCG</code> object to update <code>max1</code> (<code>int</code>) 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 <code>SUNLS_MEM_NULL</code> (<code>S</code> is <code>NULL</code>) or <code>SUNLS_SUCCESS</code> .
Deprecated Name	For backward compatibility, the wrapper function <code>SUNPCGSetMax1</code> with identical input and output arguments is also provided.
F2003 Name	<code>FSUNLinSol_PCGSetMax1</code>

8.17.3 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.

FORTTRAN 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.

FORTTRAN 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.

8.17.4 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.

8.18 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 9

Description of the SUNNonlinearSolver module

SUNDIALS time integration packages are written in terms of generic nonlinear solver operations defined by the SUNNONLINSOL API and implemented by a particular SUNNONLINSOL module of type `SUNNonlinearSolver`. Users can supply their own SUNNONLINSOL module, or use one of the modules provided with SUNDIALS. 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 9.2.

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 9.1 and proceeded to the subsequent sections in this chapter that describe the SUNNONLINSOL modules provided with SUNDIALS.

For users interested in providing their own SUNNONLINSOL module, the following section presents the SUNNONLINSOL API and its implementation beginning with the definition of SUNNONLINSOL functions in sections 9.1.1 – 9.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in section 9.1.4. A table of nonlinear solver return codes is given in section 9.1.5. The `SUNNonlinearSolver` type and the generic SUNNONLINSOL module are defined in section 9.1.6. Section 9.1.7 describes how SUNNONLINSOL models interface with SUNDIALS integrators providing sensitivity analysis capabilities (CVODES and IDAS). Finally, section 9.1.8 lists the requirements for supplying a custom SUNNONLINSOL module. Users wishing to supply their own SUNNONLINSOL module are encouraged to use the SUNNONLINSOL implementations provided with SUNDIALS as a template for supplying custom nonlinear solver modules.

9.1 The SUNNonlinearSolver API

The SUNNONLINSOL API defines several nonlinear solver operations that enable SUNDIALS integrators to utilize any SUNNONLINSOL implementation that provides the required functions. These functions can be divided into three categories. The first are the core nonlinear solver functions. The second group of functions consists of set routines to supply the nonlinear solver with functions provided by the SUNDIALS time integrators and to modify solver parameters. The final group consists of get routines for retrieving nonlinear solver statistics. All of these functions are defined in the header file `sundials/sundials_nonlinearsolver.h`.

9.1.1 SUNNonlinearSolver core functions

The core nonlinear solver functions consist of two required functions to get the nonlinear solver type (`SUNNonlinSolGetType`) 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 `SUNNonlinSolSetup` 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, callSetup, 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 9.2 for more detail on the nonlinear system formulation.

<code>y_{cor}</code>	(<code>N.Vector</code>) 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 9.2 for more detail on the nonlinear system formulation.
<code>w</code>	(<code>N.Vector</code>) the solution error weight vector used for computing weighted error norms.
<code>tol</code>	(<code>realtype</code>) the requested solution tolerance in the weighted root-mean-squared norm.
<code>callLSetup</code>	(<code>booleantype</code>) a flag indicating that the integrator recommends for the linear solver setup function to be called.
<code>mem</code>	(<code>void *</code>) the SUNDIALS integrator memory structure.

Return value The return value `retval` (of type `int`) is zero for a successful 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`

9.1.2 SUNNonlinearSolver set functions

The following set functions are used to supply nonlinear solver modules with functions defined by the SUNDIALS integrators and to modify solver parameters. Only the routine for setting the nonlinear system defining function (`SUNNonlinSolSetSysFn` is required. All other set functions are optional.

SUNNonlinSolSetSysFn

Call `retval = SUNNonlinSolSetSysFn(NLS, SysFn);`

Description The *required* function `SUNNonlinSolSetSysFn` is used to provide the nonlinear solver with the function defining the nonlinear system. This is the function $F(y)$ in $F(y) = 0$ for `SUNNONLINEARSOLVER_ROOTFIND` modules or $G(y)$ in $G(y) = y$ for `SUNNONLINEARSOLVER_FIXEDPOINT` modules.

Arguments `NLS` (`SUNNonlinearSolver`) a `SUNNONLINSOL` object.

`SysFn` (`SUNNonlinSolSysFn`) the function defining the nonlinear system. See section 9.1.4 for the definition of `SUNNonlinSolSysFn`.

Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.

F2003 Name `FSUNNonlinSolSetSysFn`

SUNNonlinSolSetLSetupFn

- Call `retval = SUNNonlinSolSetLSetupFn(NLS, LSetupFn);`
- Description The *optional* function `SUNNonlinSolSetLSetupFn` 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` (`SUNNonlinSolSetLSetupFn`) a wrapper function to the SUNDIALS integrator's linear solver setup function. See section 9.1.4 for the definition of `SUNNonlinLSetupFn`.
- Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.
- Notes The `SUNNonlinLSetupFn` function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using `SUNLINSOL` direct linear solvers) or calls the user-defined preconditioner setup function (when using `SUNLINSOL` iterative linear solvers). `SUNNONLINSOL` implementations that do not require solving this system, do not utilize `SUNLINSOL` linear solvers, or use `SUNLINSOL` linear solvers that do not require setup may set this operation to `NULL`.
- 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` (`SUNNonlinSolSetLSolveFn`) a wrapper function to the SUNDIALS integrator's linear solver solve function. See section 9.1.4 for the definition of `SUNNonlinSolSetLSolveFn`.
- 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 9.1.4 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

9.1.3 SUNNonlinearSolver get functions

The following get functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routines to get the current total number of iterations (`SUNNonlinSolGetNumIters`) and number of convergence failures (`SUNNonlinSolGetNumConvFails`) are optional. The routine to get the current nonlinear solver iteration (`SUNNonlinSolGetCurIter`) is required when using the convergence test provided by the SUNDIALS integrator or by the ARKODE and CVODE linear solver interfaces. Otherwise, `SUNNonlinSolGetCurIter` is optional.

SUNNonlinSolGetNumIters

Call `retval = SUNNonlinSolGetNumIters(NLS, numiters);`

Description The *optional* function `SUNNonlinSolGetNumIters` returns the total number of 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`

9.1.4 Functions provided by SUNDIALS integrators

To interface with `SUNNONLINSOL` modules, the SUNDIALS integrators supply a variety of routines for evaluating the nonlinear system, calling the `SUNLINSOL` setup and solve functions, and testing the nonlinear iteration for convergence. These integrator-provided routines translate between the user-supplied ODE or DAE systems and the generic interfaces to the nonlinear or linear systems of equations that result in their solution. The types for functions provided to a `SUNNONLINSOL` module are defined in the header file `sundials/sundials_nonlinearsolver.h`, and are described below.

SUNNonlinSolSysFn

- Definition `typedef int (*SUNNonlinSolSysFn)(N_Vector 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 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 9.2 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 successful solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.
- Notes As discussed in section 9.2, 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`).

`jcurn` 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 successful 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 successful 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.

9.1.5 SUNNonlinearSolver return codes

The functions provided to SUNNONLINSOL modules by each SUNDIALS integrator, and functions within the SUNDIALS-provided SUNNONLINSOL implementations utilize a common set of return codes, shown below in Table 9.1. Here, negative values correspond to non-recoverable failures, positive values to recoverable failures, and zero to a successful call.

Table 9.1: Description of the SUNNonlinearSolver return codes

Name	Value	Description
SUN-NLS_SUCCESS	0	successful call or converged solve
SUN-NLS_CONTINUE	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

9.1.6 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 9.1.1 – 9.1.3. These routines are in fact only wrappers to the nonlinear solver operations provided by a particular SUNNONLINSOL implementation, which are accessed through the ops field of the SUNNonlinearSolver structure. To illustrate this point we show below the implementation of a typical nonlinear solver operation from the generic SUNNONLINSOL module, namely SUNNonlinSolSolve, which solves the nonlinear system and returns a flag denoting a successful or failed solve:

```

int SUNNonlinSolSolve(SUNNonlinearSolver NLS,
                     N_Vector y0, N_Vector y,
                     N_Vector w, realtype tol,
                     booleantype callLSetup, void* mem)
{
  return((int) NLS->ops->solve(NLS, y0, y, w, tol, callLSetup, mem));
}

```

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

```

9.1.7 Usage with sensitivity enabled integrators

When used with SUNDIALS packages that support sensitivity analysis capabilities (e.g., CVODES and IDAS) a special NVECTOR module is used to interface with SUNNONLINSOL modules for solves involving sensitivity vectors stored in an NVECTOR array. As described below, the NVECTOR_SENSWRAPPER

module is an NVECTOR implementation where the vector content is an NVECTOR array. This wrapper vector allows SUNNONLINSOL modules to operate on data stored as a collection of vectors.

For all SUNDIALS-provided SUNNONLINSOL modules a special constructor wrapper is provided so users do not need to interact directly with the NVECTOR_SENSWRAPPER module. These constructors follow the naming convention `SUNNonlinSol_***Sens(count,...)` where `***` is the name of the SUNNONLINSOL module, `count` is the size of the vector wrapper, and `...` are the module-specific constructor arguments.

The NVECTOR_SENSWRAPPER module

This section describes the NVECTOR_SENSWRAPPER implementation of an NVECTOR. To access the NVECTOR_SENSWRAPPER module, include the header file `sundials/sundials_nvector_senswrapper.h`.

The NVECTOR_SENSWRAPPER module defines an `N_Vector` implementing all of the standard vectors operations defined in Table 6.1.1 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

$$z_{j,i} = ax_{j,i} + by_{j,i}, \quad i = 0, \dots, n-1, \quad j = 0, \dots, n_v-1.$$

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

9.1.8 Implementing a Custom SUNNonlinearSolver Module

A `SUNNONLINSOL` implementation *must* do the following:

1. Specify the content of the `SUNNONLINSOL` module.
2. Define and implement the required nonlinear solver operations defined in Sections 9.1.1 – 9.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one `SUNNONLINSOL` module (each with different `SUNNonlinearSolver` internal data representations) in the same code.
3. Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

1. Define and implement additional user-callable “set” routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.
2. Provide additional user-callable “get” routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

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`

9.2 CVODE 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

$$F(y^n) \equiv y^n - h_n \beta_{n,0} f(t_n, y^n) - a_n = 0, \quad (9.1)$$

or as the fixed-point problem

$$G(y^n) \equiv h_n \beta_{n,0} f(t_n, y^n) + a_n = y^n, \quad (9.2)$$

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 CVODE 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

$$F(y_{cor}) \equiv y_{pred} + y_{cor} - h_n \beta_{n,0} f(t_n, y_{pred} + y_{cor}) - a_n = 0, \quad (9.3)$$

for the rootfinding problem and

$$G(y_{cor}) \equiv h_n \beta_{n,0} f(t_n, y_{pred} + y_{cor}) + a_n - y_{pred} = y_{cor}. \quad (9.4)$$

for the fixed-point problem.

The nonlinear system functions provided by CVODE to the nonlinear solver module internally update the current value of the new state based on the input correction vector. The updated vector is used when calling the ODE right-hand side function and when setting up linear solves (e.g., updating the Jacobian or preconditioner).

CVODE 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.

F2003 Name `FCVodeGetCurrentGamma`

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.

F2003 Name `FCVodeGetCurrentState`

9.3 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.

9.3.1 SUNNonlinearSolver_Newton description

To find the solution to

$$F(y) = 0 \tag{9.5}$$

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

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)} \tag{9.6}$$

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

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)}), \tag{9.7}$$

in which A is the Jacobian matrix

$$A \equiv \partial F / \partial y. \tag{9.8}$$

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, 35]. 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 `SUNNonlinSolSetupFn` 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 `SUNNonlinSolSetupFn` function in two instances:

- (a) when requested by the integrator (the input `callSetSetup` 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 `SUNNonlinSolSetupFn` function.

Whether the Jacobian matrix A is fully or partially updated depends on logic unique to each integrator-supplied `SUNNonlinSolSetupFn` routine. We refer to the discussion of nonlinear solver strategies provided in Chapter 2 for details on this decision.

The default maximum number of iterations and the stopping criteria for the Newton iteration are supplied by the SUNDIALS integrator when `SUNNONLINSOL_NEWTON` is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling the `SUNNonlinSolSetMaxIters` and/or `SUNNonlinSolSetConvTestFn` functions after attaching the `SUNNONLINSOL_NEWTON` object to the integrator.

9.3.2 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 N_s sensitivities the value of `count` is:

- N_s+1 if using a *simultaneous* corrector approach.
- N_s 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 9.1.1 – 9.1.3 except for the `SUNNonlinSolSetup` function. The `SUNNONLINSOL_NEWTON` functions have the same names as those defined by the generic `SUNNONLINSOL` API with `_Newton` appended to the function name. Unless using the `SUNNONLINSOL_NEWTON` module as a standalone nonlinear solver the generic functions defined in sections 9.1.1 – 9.1.3 should be called in favor of the `SUNNONLINSOL_NEWTON`-specific implementations.

The `SUNNONLINSOL_NEWTON` module also defines the following additional user-callable function.

SUNNonlinSolGetSysFn_Newton

Call	<code>retval = SUNNonlinSolGetSysFn_Newton(NLS, SysFn);</code>
Description	The function <code>SUNNonlinSolGetSysFn_Newton</code> returns the residual function that defines the nonlinear system.
Arguments	<code>NLS</code> (<code>SUNNonlinearSolver</code>) a <code>SUNNONLINSOL</code> object <code>SysFn</code> (<code>SUNNonlinSolSysFn*</code>) the function defining the nonlinear system.
Return value	The return value <code>retval</code> (of type <code>int</code>) 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 <code>SUNNONLINSOL_NEWTON</code> module. We note that <code>SUNNONLINSOL_NEWTON</code> will not leverage the results from any user calls to <code>SysFn</code> .
F2003 Name	<code>FSUNNonlinSolGetSysFn_Newton</code>

9.3.3 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.

FORTTRAN 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.

FORTTRAN 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	<code>FSUNNEWTONINIT(code, ier);</code>
Description	The function <code>FSUNNEWTONINIT</code> can be called for Fortran programs to create a <code>SUNNonlinearSolver</code> object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ with Newton’s method.
Arguments	<code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for <code>CVODE</code> , 2 for <code>IDA</code> , and 4 for <code>ARKODE</code>).
Return value	<code>ier</code> is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

9.3.4 SUNNonlinearSolver_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.

9.4 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.

9.4.1 SUNNonlinearSolver_FixedPoint description

To find the solution to

$$G(y) = y \tag{9.9}$$

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

$$y^{(n+1)} = G(y^{(n)}) \tag{9.10}$$

where n is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [5, 45, 21, 39]. With Anderson acceleration using subspace size m , the series of approximate solutions can be formulated as the linear combination

$$y^{(n+1)} = \beta \sum_{i=0}^{m_n} \alpha_i^{(n)} G(y^{(n-m_n+i)}) + (1 - \beta) \sum_{i=0}^{m_n} \alpha_i^{(n)} y_{n-m_n+i} \tag{9.11}$$

where $m_n = \min\{m, n\}$, β is a damping parameter ($\beta = 1.0$ i.e., no damping by default) and the factors

$$\alpha^{(n)} = (\alpha_0^{(n)}, \dots, \alpha_{m_n}^{(n)}) \quad (9.12)$$

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

$$F_n = (f_{n-m_n}, \dots, f_n) \quad (9.13)$$

with $f_i = G(y^{(i)}) - y^{(i)}$. Due to this constraint, in the limit of $m = 0$ the accelerated fixed point iteration formula (9.11) simplifies to the standard fixed point iteration (9.10).

Following the recommendations made in [45], the SUNNONLINSOL_FIXEDPOINT implementation computes the series of approximate solutions as

$$y^{(n+1)} = G(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} - (1-\beta)(f(y^{(n)})) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta f_{n-m_n+i} \quad (9.14)$$

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

$$\gamma^{(n)} = (\gamma_0^{(n)}, \dots, \gamma_{m_n-1}^{(n)}) \quad (9.15)$$

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

$$\Delta F_n = (\Delta f_{n-m_n}, \dots, \Delta f_{n-1}), \quad (9.16)$$

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.

9.4.2 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 (9.10) does not require the setup or solution of any linear systems, the **SUNNONLINSOL_FIXEDPOINT** module implements all of the functions defined in sections 9.1.1 – 9.1.3 except for the **SUNNonlinSolSetup**, **SUNNonlinSolSetLSetupFn**, and **SUNNonlinSolSetLSolveFn** functions, that are set to **NULL**. The **SUNNONLINSOL_FIXEDPOINT** functions have the same names as those defined by the generic **SUNNONLINSOL** API with **_FixedPoint** appended to the function name. Unless using the **SUNNONLINSOL_FIXEDPOINT** module as a standalone nonlinear solver the generic functions defined in sections 9.1.1 – 9.1.3 should be called in favor of the **SUNNONLINSOL_FIXEDPOINT**-specific implementations.

The **SUNNONLINSOL_FIXEDPOINT** module also defines the following additional user-callable 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.

9.4.3 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	<code>FSUNFIXEDPOINTINIT(code, m, ier);</code>
Description	The function <code>FSUNFIXEDPOINTINIT</code> can be called for Fortran programs to create a <code>SUNNonlinearSolver</code> object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.
Arguments	<code>code</code> (<code>int*</code>) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, and 4 for ARKODE). <code>m</code> (<code>int*</code>) is an integer input specifying the number of acceleration vectors.
Return value	<code>ier</code> is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.

9.4.4 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.

9.5 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 libraries and *.a* for static libraries. Users of the `SUNNONLINSOL_PETSCSNES` should also see the section `NVECTOR_PETSC` [6.8](#) which discusses the `NVECTOR` interface to the PETSc Vec API.

9.5.1 `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.

9.5.2 `SUNNonlinearSolver_PetscSNES` functions

The `SUNNONLINSOL_PETSCSNES` module provides the following constructor for creating a `SUNNonlinearSolver` object.

<code>SUNNonlinSol_PetscSNES</code>

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 `sn`es (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 9.1.1 – 9.1.3 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 9.1.1 – 9.1.3 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
`snesc` (`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, PetscErrorCode* 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` (`PetscErrorCode*`) 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.

9.5.3 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 defining 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:

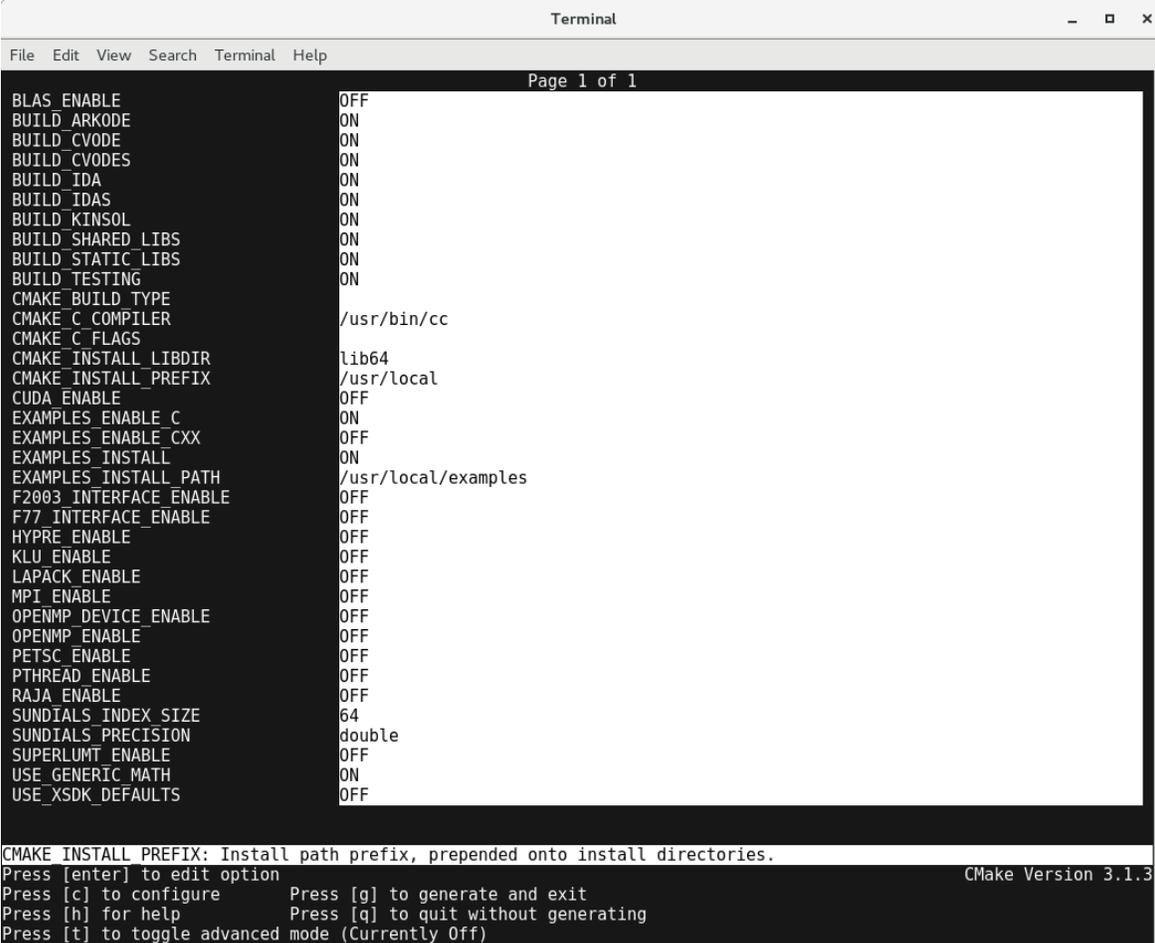
- Select and modify values, run configure (c key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
 - If it is a boolean (ON/OFF) it will toggle the value
 - If it is string or file, it will allow editing of the string

- 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.



```

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

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

```

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:

```

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

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

```

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 building 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: It 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 required 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 was built 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 desirable 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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<i>continued from last page</i>		
	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_rajah.h nvector/rajah/Vector.hpp
NVECTOR_TRILINOS	Libraries	libsundials_nvec trilinos.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
<i>continued on next page</i>		

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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_sunmatrixslunloc.lib
	Header files	sunmatrix/sunmatrix_slunloc.h
SUNMATRIX_CUSPARSE	Libraries	libsundials_sunmatrixcusparse.lib
	Header files	sunmatrix/sunmatrix_cusparse.h
SUNLINSOL_BAND	Libraries	libsundials_sunlinsolband.lib libsundials_fsunlinsolband_mod.lib libsundials_fsunlinsolband.a
	Header files	sunlinsol/sunlinsol_band.h
	Module files	fsunlinsol_band_mod.mod
SUNLINSOL_DENSE	Libraries	libsundials_sunlinsoldense.lib libsundials_fsunlinsoldense_mod.lib libsundials_fsunlinsoldense.a
	Header files	sunlinsol/sunlinsol_dense.h
	Module files	fsunlinsol_dense_mod.mod
SUNLINSOL_KLU	Libraries	libsundials_sunlinsolklu.lib libsundials_fsunlinsolklu_mod.lib libsundials_fsunlinsolklu.a
	Header files	sunlinsol/sunlinsol_klu.h
	Module files	fsunlinsol_klu_mod.mod
SUNLINSOL_LAPACKBAND	Libraries	libsundials_sunlinsollapackband.lib libsundials_fsunlinsollapackband.a
	Header files	sunlinsol/sunlinsol_lapackband.h
SUNLINSOL_LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.lib libsundials_fsunlinsollapackdense.a
	Header files	sunlinsol/sunlinsol_lapackdense.h
SUNLINSOL_PCG	Libraries	libsundials_sunlinsolpcg.lib libsundials_fsunlinsolpcg_mod.lib libsundials_fsunlinsolpcg.a
	Header files	sunlinsol/sunlinsol_pcg.h
	Module files	fsunlinsol_pcg_mod.mod
<i>continued on next page</i>		

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SUNLINSOL_SPBCGS	Libraries	libsundials_sunlinsolspbcgs. <i>lib</i> libsundials_fsunlinsolspbcgs_mod. <i>lib</i> libsundials_fsunlinsolspbcgs.a
	Header files	sunlinsol/sunlinsol_spbcgs.h
	Module files	fsunlinsol_spbcgs_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr. <i>lib</i> libsundials_fsunlinsolspgmr_mod. <i>lib</i> libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPGMR	Libraries	libsundials_sunlinsolspgmr. <i>lib</i> libsundials_fsunlinsolspgmr_mod. <i>lib</i> libsundials_fsunlinsolspgmr.a
	Header files	sunlinsol/sunlinsol_spgmr.h
	Module files	fsunlinsol_spgmr_mod.mod
SUNLINSOL_SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr. <i>lib</i> libsundials_fsunlinsolsptfqmr_mod. <i>lib</i> libsundials_fsunlinsolsptfqmr.a
	Header files	sunlinsol/sunlinsol_sptfqmr.h
	Module files	fsunlinsol_sptfqmr_mod.mod
SUNLINSOL_SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt. <i>lib</i> libsundials_fsunlinsolsuperlumt.a
	Header files	sunlinsol/sunlinsol_superlumt.h
SUNLINSOL_SUPERLUDIST	Libraries	libsundials_sunlinsolsuperludist. <i>lib</i>
	Header files	sunlinsol/sunlinsol_superludist.h
SUNLINSOL_CUSOLVERSP_BATCHQR	Libraries	libsundials_sunlinsolcusolversp. <i>lib</i>
	Header files	sunlinsol/sunlinsol_cusolverp_batchqr.h
SUNNONLINSOL_NEWTON	Libraries	libsundials_sunnonlinsolnewton. <i>lib</i> libsundials_fsunnonlinsolnewton_mod. <i>lib</i> libsundials_fsunnonlinsolnewton.a
	Header files	sunnonlinsol/sunnonlinsol_newton.h
	Module files	fsunnonlinsol_newton_mod.mod
SUNNONLINSOL_FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint. <i>lib</i> libsundials_fsunnonlinsolfixedpoint.a libsundials_fsunnonlinsolfixedpoint_mod. <i>lib</i>
	Header files	sunnonlinsol/sunnonlinsol_fixedpoint.h
	Module files	fsunnonlinsol_fixedpoint_mod.mod
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SUNNONLINSOL_PETSCSNES	Libraries	libsundials_sunnonlinsolpetscsnes. <i>lib</i>	
	Header files	sunnonlinsol/sunnonlinsol_petscsnes.h	
CVODE	Libraries	libsundials_cvode. <i>lib</i> libsundials_fcvcde.a libsundials_fcvcde_mod. <i>lib</i>	
	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	fcvcde_mod.mod	
CVODES	Libraries	libsundials_cvodes. <i>lib</i> libsundials_fcvcodes_mod. <i>lib</i>	
	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	fcvcodes_mod.mod	
ARKODE	Libraries	libsundials_arkode. <i>lib</i> libsundials_farkode.a libsundials_farkode_mod. <i>lib</i>	
	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_mrstep_mod.mod
IDA	Libraries	libsundials_ida. <i>lib</i> libsundials_fida.a libsundials_fida_mod. <i>lib</i>	
	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. <i>lib</i> libsundials_fidas_mod. <i>lib</i>	
	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	
<i>continued on next page</i>			

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KINSOL	Libraries	libsundials_kinsol. <i>lib</i> libsundials_fkinsol.a libsundials_fkinsol_mod. <i>lib</i>
	Header files	kinsol/kinsol.h kinsol/kinsol_impl.h kinsol/kinsol_direct.h kinsol/kinsol_ls.h kinsol/kinsol_spils.h kinsol/kinsol_bbdpre.h
	Module files	fkinsol_mod.mod

Appendix B

CVODE 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 CVODE input constants

CVODE 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.

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 CVODE output constants

CVODE 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 <code>mxstep</code> 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 repeated 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 <code>cvode_mem</code> 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 <code>CVodeMalloc</code> .
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.

CVLS linear solver interface

CVLS_SUCCESS	0	Successful function return.
CVLS_MEM_NULL	-1	The <code>cvode_mem</code> 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.
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.

CVDIAG linear solver module

CVDIAG_SUCCESS	0	Successful function return.
CVDIAG_MEM_NULL	-1	The <code>cvode_mem</code> 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.

Appendix C

SUNDIALS Release History

Table C.1: Release History

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Mar 2020	5.2.0	4.2.0	5.2.0	5.2.0	5.2.0	4.2.0	5.2.0
Jan 2020	5.1.0	4.1.0	5.1.0	5.1.0	5.1.0	4.1.0	5.1.0
Oct 2019	5.0.0	4.0.0	5.0.0	5.0.0	5.0.0	4.0.0	5.0.0
Feb 2019	4.1.0	3.1.0	4.1.0	4.1.0	4.1.0	3.1.0	4.1.0
Jan 2019	4.0.2	3.0.2	4.0.2	4.0.2	4.0.2	3.0.2	4.0.2
Dec 2018	4.0.1	3.0.1	4.0.1	4.0.1	4.0.1	3.0.1	4.0.1
Dec 2018	4.0.0	3.0.0	4.0.0	4.0.0	4.0.0	3.0.0	4.0.0
Oct 2018	3.2.1	2.2.1	3.2.1	3.2.1	3.2.1	2.2.1	3.2.1
Sep 2018	3.2.0	2.2.0	3.2.0	3.2.0	3.2.0	2.2.0	3.2.0
Jul 2018	3.1.2	2.1.2	3.1.2	3.1.2	3.1.2	2.1.2	3.1.2
May 2018	3.1.1	2.1.1	3.1.1	3.1.1	3.1.1	2.1.1	3.1.1
Nov 2017	3.1.0	2.1.0	3.1.0	3.1.0	3.1.0	2.1.0	3.1.0
Sep 2017	3.0.0	2.0.0	3.0.0	3.0.0	3.0.0	2.0.0	3.0.0
Sep 2016	2.7.0	1.1.0	2.9.0	2.9.0	2.9.0	1.3.0	2.9.0
Aug 2015	2.6.2	1.0.2	2.8.2	2.8.2	2.8.2	1.2.2	2.8.2
Mar 2015	2.6.1	1.0.1	2.8.1	2.8.1	2.8.1	1.2.1	2.8.1
Mar 2015	2.6.0	1.0.0	2.8.0	2.8.0	2.8.0	1.2.0	2.8.0
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

continued on next page

<i>continued from last page</i>							
Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Mar 2005	2.0.2	–	2.2.2	2.1.2	2.2.2	–	2.2.2
Jan 2005	2.0.1	–	2.2.1	2.1.1	2.2.1	–	2.2.1
Dec 2004	2.0.0	–	2.2.0	2.1.0	2.2.0	–	2.2.0
Jul 2002	1.0.0	–	2.0.0	1.0.0	2.0.0	–	2.0.0
Mar 2002	–	–	1.0.0 ³	–	–	–	–
Feb 1999	–	–	–	–	1.0.0 ⁴	–	–
Aug 1998	–	–	–	–	–	–	1.0.0 ⁵
Jul 1997	–	–	1.0.0 ²	–	–	–	–
Sep 1994	–	–	1.0.0 ¹	–	–	–	–

¹CVODE written, ²PVODE written, ³CVODE and PVODE combined, ⁴IDA written, ⁵KINSOL written

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