

# User Documentation for CVODE v4.0.0-dev.1 (SUNDIALS v4.0.0-dev.1)

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# Chapter 1

## Introduction

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

### 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 [5] and VODPK [8]. 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 [33]. 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 [6]. The capabilities of both VODE and VODPK have been combined in the C-language package CVODE [13].

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) [36], FGMRES (Flexible Generalized Minimum RESidual) [35], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [37], TFQMR (Transpose-Free Quasi-Minimal Residual) [19], and PCG (Preconditioned Conjugate Gradient) [20] 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 PVIDE [11], 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 Hydre 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 v4.0.0-dev.1

An API for encapsulating the nonlinear solvers used in SUNDIALS implicit integrators has been introduced. The goal of this API is to ease the introduction of new nonlinear solver options in SUNDIALS integrators and allow for external or user-supplied nonlinear solvers. The SUNNONLINSOL API and provided SUNNONLINSOL modules are described in Chapter 9 and follow the same object oriented design and implementation used by the NVECTOR, SUNMATRIX, and SUNLINSOL modules.

SUNNONLINSOL modules are intended to solve nonlinear systems formulated as either a rootfinding problem  $F(y) = 0$  or a fixed-point problem  $G(y) = y$ . 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. Additionally, the fixed-point iteration can use Anderson's method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all CVODE 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 as well as 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 CVODE memory structure, CVODE uses the SUNNONLINSOL\_NEWTON module implementation of a Newton iteration by default. To use the fixed-point nonlinear solver with CVODE a user must do the following:

1. include the header `sunnonlinsol/sunnonlinsol_fixedpoint.h` to access the `SUNNONLINSOL_FIXEDPOINT` module,
2. create a nonlinear solver object by calling the fixed-point constructor

```
NLS = SUNNonlinSol_FixedPoint(y, m);
```

where `NLS` is the nonlinear solver object of type `SUNNonlinearSolver`, `y` is an `NVector` the size of the ODE system, and `m` is the number of acceleration vectors (see §9.3 for more detail), and

3. after initializing CVODE with `CVodeInit`, call

```
retval = CVodeSetNonlinearSolver(cvode_mem, NLS);
```

to attach the nonlinear solver object to the CVODE memory structure.

User-supplied nonlinear solver modules adhering to the SUNNONLINSOL API for solving  $F(y) = 0$  or  $G(y) = y$  can be used with CVODE by following the same include, create, and attach process just described for the SUNNONLINSOL\_FIXEDPOINT module.

As a result of this new nonlinear solver object creation and attachment approach, the function `CVodeSetIterType` has been removed. CVODE 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.

## Changes in v4.0.0-dev

Three fused vector operations and seven vector array operations have been added to the NVECTOR API. These *optional* 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 new operations are `N_VLinearCombination`, `N_VScaleAddMulti`, `N_VDotProdMulti`, `N_VLinearCombinationVectorArray`, `N_VScaleVectorArray`, `N_VConstVectorArray`, `N_VWrmsNormVectorArray`, `N_VWrmsNormMaskVectorArray`, `N_VScaleAddMultiVectorArray`, and `N_VLinearCombinationVectorArray`. If any of these operations are defined as NULL in an NVECTOR implementation the NVECTOR interface will automatically call standard NVECTOR operations as necessary. Details on the new operations can be found in Chapter 6.

Several changes were made to the build system. 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 native CMake FindMPI module is now used to locate an MPI installation. The options for setting MPI compiler wrappers and the executable for running MPI programs have been updated to align with those in native CMake FindMPI module. This included changing `MPI_MPICC` to `MPI_C_COMPILER`, `MPI_MPICXX` to `MPI_CXX_COMPILER`, combining `MPI_MPIF77` and `MPI_MPIF90` to `MPI_Fortran_COMPILER`, and changing `MPI_RUN_COMMAND` to `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. Additionally, 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 SUNLINEARSOLVER module to use a `typedef` for the precision-specific solve function to be used (to avoid compiler warnings).
- Added missing typecasts for some (`void*`) pointers (again, to avoid compiler warnings).
- Bugfix in `sunmatrix_sparse.c` where we had used `int` instead of `sunindextype` in one location.
- Added missing `#include <stdio.h>` in NVECTOR and SUNMATRIX header files.
- 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, `NVGetVectorID`, 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 `linit` 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`, `SUNRpowerI`, 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 `strncmpp` 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 [27].

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 FCVODE, an interface module for 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 (§7.1), a banded implementation (§7.2) and a sparse implementation (§7.3).
- 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 CVDLS, 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 [12] and George D. Byrne [10].

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## 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  $K_2 = q$  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 [9] and [29].

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 §9.2. 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 [3, 38, 18, 32] to accelerate convergence (see §9.3 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 [14, 1], or the thread-enabled SuperLU\_MT sparse solver library [31, 16, 2] (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 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 [6].

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 cases of a direct solver (dense, band, sparse, or diagonal), the default Newton iteration is a Modified Newton iteration, in that the iteration matrix  $M$  is fixed throughout the nonlinear iterations. However, for any of the Krylov methods, it 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  $M$  (direct cases) or preconditioner matrix  $P$  (Krylov cases) is 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  $\gamma$  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  $\gamma$  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  $\epsilon$ , specifically that it is less than  $0.1\epsilon$ . (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 a Krylov 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  $\delta_m$  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  $0.05 \cdot (0.1\epsilon)$ .

With the direct dense and band methods, 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  $\sigma_j$  are given by

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

where  $U$  is the unit roundoff,  $\sigma_0$  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 the sparse direct solvers, 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  $\sigma$  is  $1/\|v\|$ , so that  $\sigma v$  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 [5, 8, 24]. They are also summarized in [25].

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, these solvers are rarely successful if used without preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system  $Ax = b$  can be preconditioned on the left, as  $(P^{-1}A)x = P^{-1}b$ ; on the right, as  $(AP^{-1})Px = b$ ; or on both sides, as  $(P_L^{-1}AP_R^{-1})P_Rx = P_L^{-1}b$ . The Krylov method is then applied to a system with the matrix  $P^{-1}A$ , or  $AP^{-1}$ , or  $P_L^{-1}AP_R^{-1}$ , instead of  $A$ . In order to improve the convergence of the Krylov iteration, the preconditioner matrix  $P$ , or the product  $P_LP_R$  in the last case, should in some sense approximate the system matrix  $A$ . Yet at the same time, in order to be cost-effective, the matrix  $P$ , or matrices  $P_L$  and  $P_R$ , should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [6] 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  $P_LP_R$ ). 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  $\lambda$  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  $\lambda$  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  $\nu$  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 [22]. 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 [23], 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 [21]. 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  $\delta$ , 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  $\alpha$  is a weight parameter. On the first two passes through the loop,  $\alpha$  is set to 1, making  $t_{mid}$  the secant method value. Thereafter,  $\alpha$  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,  $\alpha$  is set to 1. If the two sides were the same,  $\alpha$  is halved (if on the low side) or doubled (if on the high side). The value of  $t_{mid}$  is closer to  $t_{lo}$  when  $\alpha < 1$  and closer to  $t_{hi}$  when  $\alpha > 1$ . If the above value of  $t_{mid}$  is within  $\tau/2$  of  $t_{lo}$  or  $t_{hi}$ , it is adjusted inward, such that its fractional distance from the endpoint (relative to the interval size) is between .1 and .5 (.5 being the midpoint), and the actual distance from the endpoint is at least  $\tau/2$ .



# Chapter 3

## Code Organization

### 3.1 SUNDIALS organization

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

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see Figs. 3.1 and 3.2). The following is a list of the solver packages presently available, and the basic functionality of each:

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

### 3.2 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 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 *direct* linear solver interface, CVDLS, supports SUNLINSOL implementations with type `SUNLINSOL_DIRECT` (see Chapter 8). These linear solvers utilize direct methods for the solution of linear systems stored using one of the SUNDIALS generic SUNMATRIX implementations (dense, banded or sparse; see Chapter 7). It is assumed that the

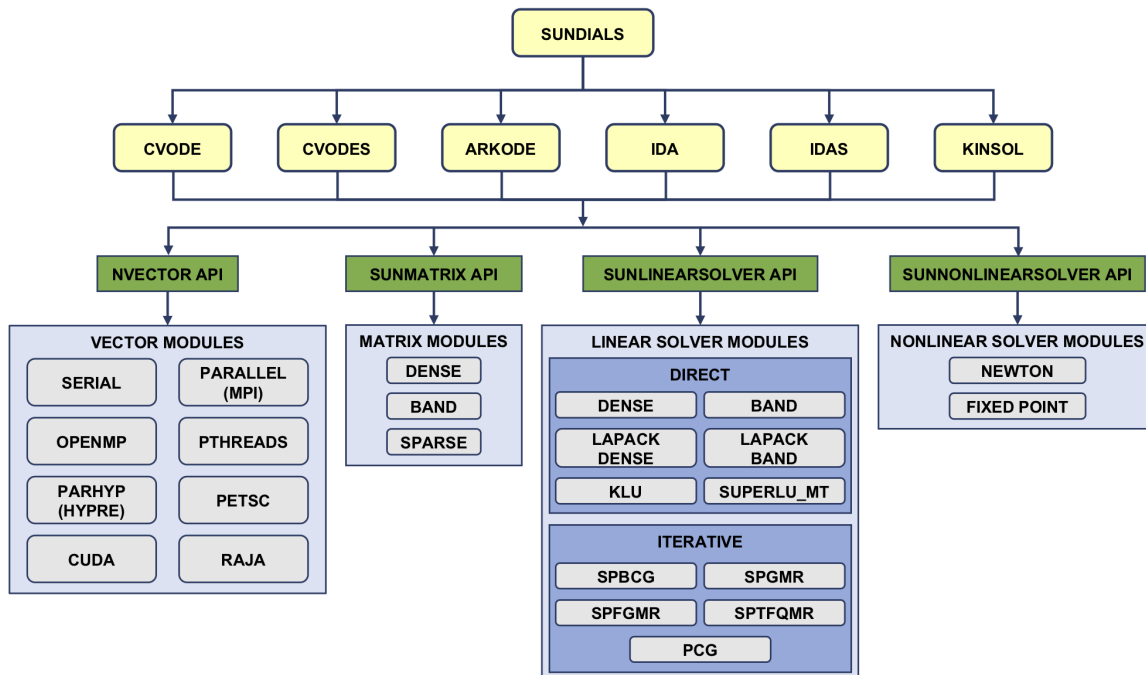


Figure 3.1: High-level diagram of the SUNDIALS suite

dominant cost for such solvers occurs in factorization of the linear system matrix  $M$ , so the `SUNNONLINEAR_SOLVE_NEWTON` module utilizes these solvers within a modified Newton nonlinear solve. The *spils* linear solver interface, `CVSPILS`, supports `SUNLINSOL` implementations with type `SUNLINSOL_ITERATIVE` (see Chapter 8). These linear solvers utilize scaled preconditioned iterative methods. It is assumed that these methods are implemented in a “matrix-free” manner, wherein only the action of the matrix-vector product  $Mv$  is required. Since `CVODE` can operate on any valid `SUNLINSOL` implementation of `SUNLINSOL_DIRECT` or `SUNLINSOL_ITERATIVE` types, the set of linear solver modules available to `CVODE` will expand as new `SUNLINSOL` modules are developed.

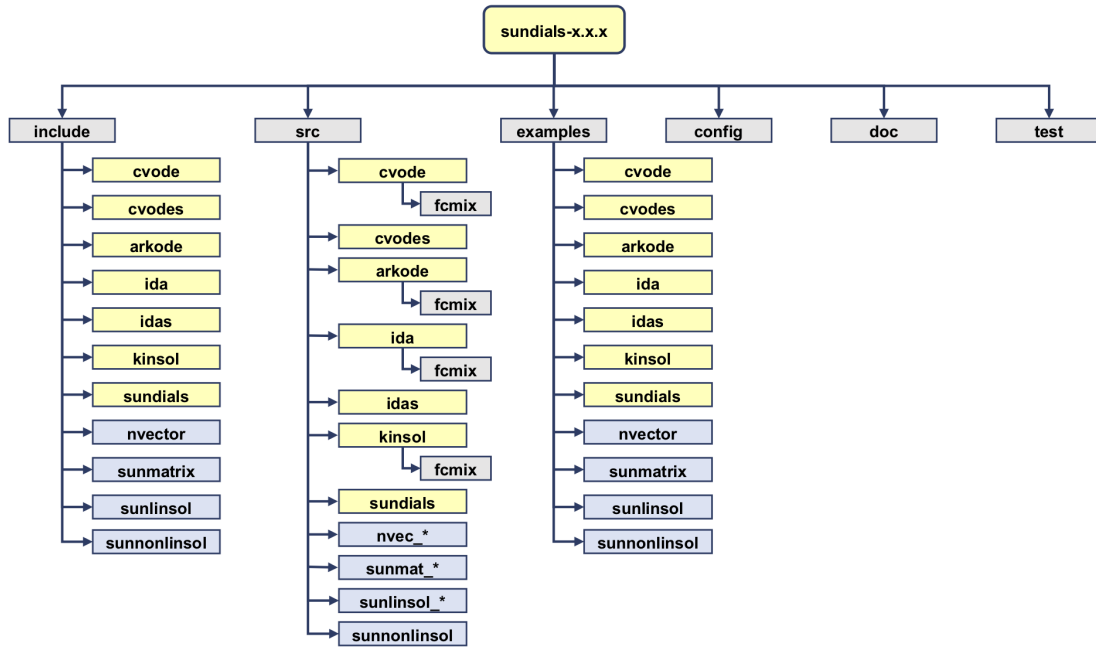
Additionally, `CVODE` includes the *diagonal* linear solver interface, `CVDIAG`, that creates an internally generated diagonal approximation to the Jacobian.

Within the `CVDLS` interface, the package includes algorithms for the approximation of dense or banded Jacobians through difference quotients, but the user also has the option of supplying the Jacobian (or an approximation to it) directly. This user-supplied routine is required when using sparse Jacobian matrices, since standard difference quotient approximations do not leverage the inherent sparsity of the problem.

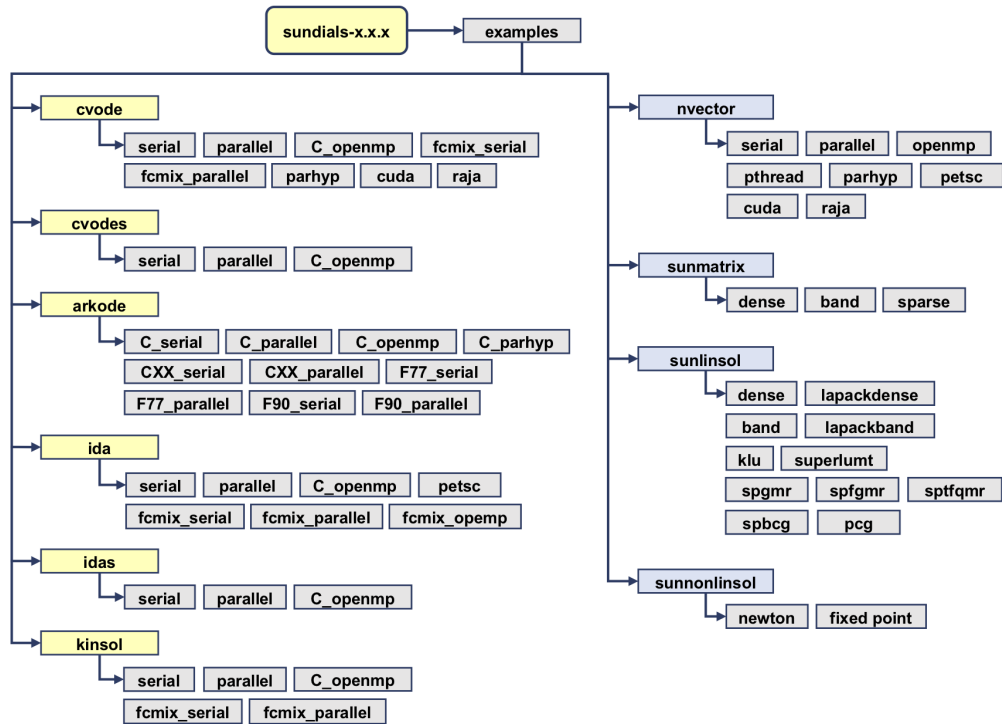
Within the `CVSPILS` interface, the package includes an algorithm for the approximation by difference quotients of the product  $Mv$ . Again, the user has the option of providing routines for this operation, in two phases: setup (preprocessing of Jacobian data) and multiplication. For preconditioned 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 [6, 8], together with the example and demonstration programs included with `CVODE`, offer considerable assistance in building preconditioners.

Each `CVODE` 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.





(a) Directory structure of the SUNDIALS source tree



(b) Directory structure of the SUNDIALS examples

Figure 3.2: Organization of the SUNDIALS suite

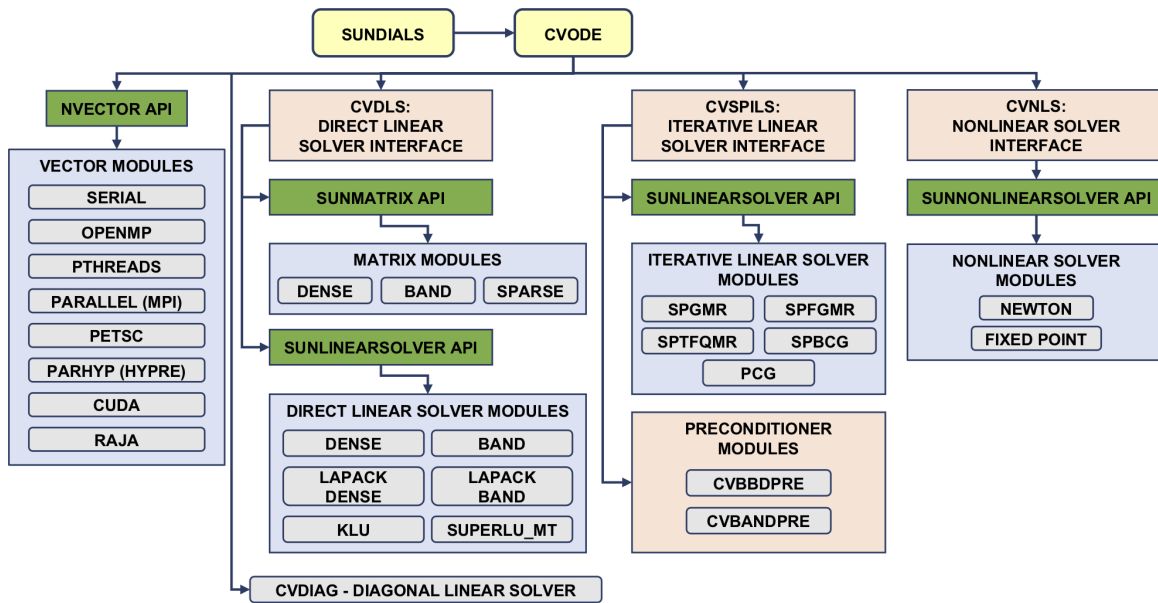


Figure 3.3: Overall structure diagram of the CVODE package. Modules specific to CVODE begin with “CV” (CVDLS, CVDIAG, CVSPILS, CVBBDPRE, CVBANDPRE, and CVNLS), all other items correspond to generic solver and auxiliary modules. Note also that the LAPACK, KLU and SUPERLUMT support is through interfaces to external packages. Users will need to download and compile those packages independently.

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 [27] 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 the FORTRAN/C interface module.

The user should be aware that not all SUNLINSOL and SUNMATRIX modules are compatible with all NVECTOR implementations. Details on compatability 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 compatability 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* (one to four files),

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.

A user program which uses the type `realtype` and the `RCONST` macro to handle floating-point constants is precision-independent except for any calls to precision-specific standard math library functions. (Our example programs use both `realtype` and `RCONST`.) Users can, however, use the type `double`, `float`, or `long double` in their code (assuming that this usage is consistent with the typedef for `realtype`). Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use `realtype`, so long as the SUNDIALS libraries use the correct precision (for details see §A.1.2).

### 4.2.2 Integer types used for vector and matrix indices

The type `sunindextype` can be either a 32- or 64-bit *signed* integer. The default is the portable `int64_t` type, and the user can change it to `int32_t` at the configuration stage. The configuration system will detect if the compiler does not support portable types, and will replace `int32_t` and `int64_t` with `int` and `long int`, respectively, to ensure use of the desired sizes on Linux, Mac OS X, and Windows platforms. SUNDIALS currently does not support *unsigned* integer types for vector and matrix indices, although these could be added in the future if there is sufficient demand.

A user program which uses `sunindextype` to handle vector and matrix indices will work with both index storage types except for any calls to index storage-specific external libraries. (Our C and C++ example programs use `sunindextype`.) Users can, however, use any one of `int`, `long int`, `int32_t`, `int64_t` or `long long int` in their code, assuming that this usage is consistent with the typedef for `sunindextype` on their architecture). Thus, a previously existing piece of ANSI C code can use SUNDIALS without modifying the code to use `sunindextype`, so long as the SUNDIALS libraries use the appropriate index storage type (for details see §A.1.2).

## 4.3 Header files

The calling program must include several header files so that various macros and data types can be used. The header file that is always required is:

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

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

The calling program must also include a 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`. See Chapter 9 for the appropriate name. 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 linear solver interfaces and linear solver modules available for use with CVODE are:

- `cvode/cvode_direct.h`, which is used with the CVDLS direct linear solver interface to access direct solvers with the following header files:
  - `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 interface module, `SUNLINSOL_LAPACKDENSE`;
  - `sunlinsol/sunlinsol_lapackband.h`, which is used with the LAPACK banded linear solver interface module, `SUNLINSOL_LAPACKBAND`;
  - `sunlinsol/sunlinsol_klu.h`, which is used with the KLU sparse linear solver interface module, `SUNLINSOL_KLU`;
  - `sunlinsol/sunlinsol_superlunt.h`, which is used with the SUPERLUNT sparse linear solver interface module, `SUNLINSOL_SUPERLUNT`;
- `cvode/cvode_spils.h`, which is used with the CVSPILS iterative linear solver interface to access iterative solvers with the following header files:
  - `sunlinsol/sunlinsol_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver module, `SUNLINSOL_SPGMR`;
  - `sunlinsol/sunlinsol_spfgmr.h`, which is used with the scaled, preconditioned FGMRES Krylov linear solver module, `SUNLINSOL_SPFGMR`;

- `sunlinsol/sunlinsol.spbcgs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, `SUNLINSOL_SPBCGS`;
- `sunlinsol/sunlinsol.sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov linear solver module, `SUNLINSOL_SPTFQMR`;
- `sunlinsol/sunlinsol.pcg.h`, which is used with the scaled, preconditioned CG Krylov linear solver module, `SUNLINSOL_PCG`;
- `cvode/cvode_diag.h`, which is used with the `CVDIAG` diagonal linear solver interface.

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 [27]), preconditioning is done with a block-diagonal matrix. For this, even though the `SUNLINSOL_SPGMR` linear solver is used, the header `sundials/sundials_dense.h` is included for access to the underlying generic dense matrix arithmetic routines.

## 4.4 A skeleton of the user's main program

The following is a skeleton of the user's main program (or calling program) for the integration of an ODE IVP. Most of the steps are independent of the `NVECTOR`, `SUNMATRIX`, and `SUNLINSOL` implementations used. For the steps that are not, refer to Chapters 6, 7, and 8 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 §6.1-6.4 for details.

For the `hypr` 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 §6.5 and §6.6 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 §6.7-6.8 for details.

#### 4. Create CVMODE object

Call `cvmode_mem = CVMODECreate(lmm)` to create the CVMODE memory block and to specify the solution method (linear multistep method). `CVMODECreate` returns a pointer to the CVMODE memory structure. See §4.5.1 for details.

#### 5. Initialize CVMODE solver

Call `CVMODEInit(...)` to provide required problem specifications, allocate internal memory for CVMODE, and initialize CVMODE. `CVMODEInit` 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 `CVMODESStolerances(...)` or `CVMODESVtolerances(...)` 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 `CVMODEWftolerances` to specify a function which sets directly the weights used in evaluating WRMS vector norms. See §4.5.2 for details.

#### 7. Set optional inputs

Call `CVMODESet*` functions to change any optional inputs that control the behavior of CVMODE from their default values. See §4.5.7.1 for details.

#### 8. Create matrix object

If a nonlinear solver requiring a linear solve will be used (e.g., the the default Newton iteration) and the linear solver will be a direct linear solver, then a template Jacobian matrix must be created by calling the appropriate constructor function defined by the particular SUNMATRIX implementation.

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

#### 9. 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.

#### 10. 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.

#### 11. Attach linear solver module

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

```
ier = CVDlsSetLinearSolver(...);
ier = CVSpilsSetLinearSolver(...);
```

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(...);
```

#### 12. Set linear solver interface optional inputs

Call `CVDlsSet*` or `CVSpilsSet*` functions to change optional inputs specific to that linear solver interface. See §4.5.7 for details.

#### 13. Create nonlinear solver object (*optional*)

If using a non-default nonlinear solver, 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).

#### 14. Attach nonlinear solver module (*optional*)

If using a non-default nonlinear solver, then initialize the `CVNLS` nonlinear solver interface by attaching the nonlinear solver object by calling `ier = CVodeSetNonlinearSolver(cvode_mem, NLS)`;

#### 15. 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.

#### 16. 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 §4.5.7.4 for relevant optional input calls.

#### 17. 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.

#### 18. Get optional outputs

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

#### 19. 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);
```

#### 20. Free solver memory

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

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

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

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

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



### 23. Finalize MPI, if used

Call `MPI_Finalize()` to terminate MPI.

SUNDIALS provides some linear solvers only as a means for users to get problems running and not as highly efficient solvers. For example, if solving a dense system, we suggest using the LAPACK solvers if the size of the linear system is  $> 50,000$ . (Thanks to A. Nicolai for his testing and recommendation.) Table 4.1 shows the linear solver interfaces available as SUNLINSOL modules and the vector implementations required for use. As an example, one cannot use the dense direct solver interfaces with the MPI-based vector implementation. However, as discussed in Chapter 8 the SUNDIALS packages operate on generic SUNLINSOL objects, allowing a user to develop their own solvers should they so desire.

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

Linear Solver	Serial	Parallel (MPI)	OpenMP	pThreads	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`.

#### 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.

#### 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.

### 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.

#### 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**.

#### CVodeWftolerances

Call **flag** = **CVodeWftolerances**(**cvode\_mem**, **efun**);

Description The function **CVodeWftolerances** specifies a user-supplied function **efun** that sets the multiplicative error weights  $W_i$  for use in the weighted RMS norm, which are normally defined by Eq. (2.7).

Arguments **cvode\_mem** (**void \***) pointer to the CVODE memory block returned by **CVodeCreate**.  
**efun** (**CVWtFn**) is the C function which defines the **ewt** vector (see §4.6.3).

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

- CV\_SUCCESS** The call to **CVodeWftolerances** was successful.
- CV\_MEM\_NULL** The CVODE memory block was not initialized through a previous call to **CVodeCreate**.
- CV\_NO\_MALLOC** The allocation function **CVodeInit** has not been called.

**General advice on choice of tolerances.** For many users, the appropriate choices for tolerance values in **reltol** and **abstol** are a concern. The following pieces of advice are relevant.

(1) The scalar relative tolerance **reltol** is to be set to control relative errors. So **reltol** =  $10^{-4}$  means that errors are controlled to .01%. We do not recommend using **reltol** larger than  $10^{-3}$ . On the other hand, **reltol** should not be so small that it is comparable to the unit roundoff of the machine arithmetic (generally around  $1.0\text{E-}15$ ).

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

(3) Finally, it is important to pick all the tolerance values conservatively, because they control the error committed on each individual time step. The final (global) errors are 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 three CVODE linear solver interfaces currently available for this task: `CVDLS`, `CVDIAG` and `CVSPILS`.

The first corresponds to the use of Direct Linear Solvers, and utilizes `SUNMATRIX` objects to store the Jacobian  $J = \partial f / \partial y$ , the matrix  $M = I - \gamma J$ , and factorizations used throughout the solution process.

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

The third corresponds to the use of Scaled, Preconditioned, Iterative Linear Solvers, utilizing matrix-free Krylov methods to solve the linear systems of equations. With most of these methods, preconditioning can be done on the left only, on the right only, on both the left and the right, or not at all. The exceptions to this rule are `SPFGMR` that supports right preconditioning only and `PCG` that performs symmetric preconditioning. 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 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).

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 SUNLINSOL object and call either of the functions `CVDlsSetLinearSolver` or `CVSpilsSetLinearSolver`, as documented below. The first argument passed to these functions is the CVODE memory pointer returned by `CVodeCreate`; the second argument passed to these functions is the desired SUNLINSOL object to use for solving linear systems. A call to one of these functions initializes the appropriate CVODE linear solver interface, linking this to the main CVODE integrator, and allows the user to specify parameters which are specific to a particular solver interface. The use of each of the generic linear solvers involves certain constants 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.

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

#### `CVDlsSetLinearSolver`

Call	<code>flag = CVDlsSetLinearSolver(cvode_mem, LS, J);</code>
Description	<p>The function <code>CVDlsSetLinearSolver</code> attaches a direct SUNLINSOL object <code>LS</code> and corresponding template Jacobian SUNMATRIX object <code>J</code> to CVODE, initializing the CVDLS direct linear solver interface.</p> <p>The user's main program must include the <code>cvode_direct.h</code> header file.</p>
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>LS</code> (<code>SUNLinearSolver</code>) SUNLINSOL object to use for solving linear systems of the form (2.5).</p> <p><code>J</code> (<code>SUNMatrix</code>) SUNMATRIX object for used as a template for the Jacobian (must have a type compatible with the linear solver object).</p>
Return value	<p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVDLS_SUCCESS</code> The CVDLS initialization was successful.</p> <p><code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</p> <p><code>CVDLS_ILL_INPUT</code> The CVDLS solver is not compatible with the <code>LS</code> or <code>J</code> input objects or is incompatible with the current NVECTOR module.</p> <p><code>CVDLS_MEM_FAIL</code> A memory allocation request failed.</p>
Notes	<p>The CVDLS linear solver interface is not compatible with all implementations of the SUNLINSOL and NVECTOR modules. Specifically, CVDLS requires use of a <i>direct</i> SUNLINSOL object and a serial or threaded NVECTOR module. Additional compatibility limitations for each SUNLINSOL object (i.e. SUNMATRIX and NVECTOR object compatibility) are described in Chapter 8.</p>

#### `CVSpilsSetLinearSolver`

Call	<code>flag = CVSpilsSetLinearSolver(cvode_mem, LS);</code>
Description	<p>The function <code>CVSpilsSetLinearSolver</code> attaches an iterative SUNLINSOL object <code>LS</code> to CVODE, initializing the CVSPILS scaled, preconditioned, iterative linear solver interface.</p> <p>The user's main program must include the <code>cvode_spils.h</code> header file.</p>
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>LS</code> (<code>SUNLinearSolver</code>) SUNLINSOL object to use for solving linear systems of the form (2.5).</p>
Return value	<p>The return value <code>flag</code> (of type <code>int</code>) is one of</p>

CVSPILS\_SUCCESS The CVSPILS initialization was successful.  
 CVSPILS\_MEM\_NULL The `cvoice_mem` pointer is NULL.  
 CVSPILS\_ILL\_INPUT The CVSPILS solver is not compatible with the LS object or is incompatible with the current NVECTOR module.  
 CVSPILS\_MEM\_FAIL A memory allocation request failed.  
 CVSPILS\_SUNLS\_FAIL A call to the LS object failed.

Notes The CVSPILS linear solver interface is not compatible with all implementations of the SUNLINSOL and NVECTOR modules. Specifically, CVSPILS requires use of an *iterative* SUNLINSOL object. Additional compatibility limitations for each SUNLINSOL object (i.e. required NVECTOR routines) are described in Chapter 8.

#### CVDiag

Call `flag = CVDiag(cvoice_mem);`

Description The function `CVDiag` selects the CVDIAG linear solver.  
 The user's main program must include the `cvoice_diag.h` header file.

Arguments `cvoice_mem` (`void *`) pointer to the CVOICE 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 `cvoice_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 current CVOICE linear solver interfaces. The CVDIAG solver uses an approximate diagonal Jacobian formed by way of a difference quotient. The user does *not* have the option of supplying a function to compute an approximate diagonal Jacobian.

### 4.5.4 Nonlinear solver interface function

By default CVOICE uses the SUNNONLINSOL implementation of Newton's method defined by the SUNNONLINSOL\_NEWTON module (see §9.2). To specify a different nonlinear solver in CVOICE, the user's program must create a SUNNONLINSOL object by calling the appropriate constructor routine and attach the SUNNONLINSOL object by calling `CVodeSetNonlinearSolver`, as documented below.

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

The first argument passed to `CVodeSetNonlinearSolver` is the CVOICE 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 CVOICE integrator.

#### CVodeSetNonlinearSolver

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

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

Arguments `cvoice_mem` (`void *`) pointer to the CVOICE memory block.

LS (`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.

#### 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`.

#### 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:

<code>CV_SUCCESS</code>	<code>CVode</code> succeeded and no roots were found.
<code>CV_TSTOP_RETURN</code>	<code>CVode</code> succeeded by reaching the stopping point specified through the optional input function <code>CVodeSetStopTime</code> (see §4.5.7.1).
<code>CV_ROOT_RETURN</code>	<code>CVode</code> succeeded and found one or more roots. In this case, <code>tret</code> is the location of the root. If <code>nrtfn &gt; 1</code> , call <code>CVodeGetRootInfo</code> to see which $g_i$ were found to have a root.
<code>CV_MEM_NULL</code>	The <code>cvode_mem</code> argument was <code>NULL</code> .
<code>CV_NO_MALLOC</code>	The <code>CVODE</code> memory was not allocated by a call to <code>CVodeInit</code> .
<code>CV_ILL_INPUT</code>	One of the inputs to <code>CVode</code> 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 <code>CVodeCreate</code> ) failed to set the linear solver-specific <code>lsolve</code> field in <code>cvode_mem</code> . (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.
<code>CV_TOO_CLOSE</code>	The initial time $t_0$ and the final time $t_{out}$ are too close to each other and the user did not specify an initial step size.
<code>CV_TOO_MUCH_WORK</code>	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> .
<code>CV_TOO_MUCH_ACC</code>	The solver could not satisfy the accuracy demanded by the user for some internal step.
<code>CV_ERR_FAILURE</code>	Either error test failures occurred too many times ( <code>MXNEF = 7</code> ) during one internal time step, or with $ h  = h_{min}$ .
<code>CV_CONV_FAILURE</code>	Either convergence test failures occurred too many times ( <code>MXNCF = 10</code> ) during one internal time step, or with $ h  = h_{min}$ .
<code>CV_LINIT_FAIL</code>	The linear solver's initialization function failed.
<code>CV_LSETUP_FAIL</code>	The linear solver's setup function failed in an unrecoverable manner.
<code>CV_LSOLVE_FAIL</code>	The linear solver's solve function failed in an unrecoverable manner.
<code>CV_RHSFUNC_FAIL</code>	The right-hand side function failed in an unrecoverable manner.
<code>CV_FIRST_RHSFUNC_FAIL</code>	The right-hand side function had a recoverable error at the first call.
<code>CV_REPTD_RHSFUNC_ERR</code>	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.
<code>CV_UNREC_RHSFUNC_ERR</code>	The right-hand side 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.
<code>CV_RTFUNC_FAIL</code>	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`.



Table 4.2: Optional inputs for CVODE, CVDLS, and CVSPILS

Optional input	Function name	Default
<b>CVODE main solver</b>		
Pointer to an error file	CVodeSetErrFile	stderr
Error handler function	CVodeSetErrHandlerFn	internal fn.
User data	CVodeSetUserData	NULL
Maximum order for BDF method	CVodeSetMaxOrd	5
Maximum order for Adams method	CVodeSetMaxOrd	12
Maximum no. of internal steps before $t_{\text{out}}$	CVodeSetMaxNumSteps	500
Maximum no. of warnings for $t_n + h = t_n$	CVodeSetMaxHnilWarns	10
Flag to activate stability limit detection	CVodeSetStabLimDet	SUNFALSE
Initial step size	CVodeSetInitStep	estimated
Minimum absolute step size	CVodeSetMinStep	0.0
Maximum absolute step size	CVodeSetMaxStep	$\infty$
Value of $t_{\text{stop}}$	CVodeSetStopTime	undefined
Maximum no. of error test failures	CVodeSetMaxErrTestFails	7
Maximum no. of nonlinear iterations	CVodeSetMaxNonlinIters	3
Maximum no. of convergence failures	CVodeSetMaxConvFails	10
Coefficient in the nonlinear convergence test	CVodeSetNonlinConvCoef	0.1
Direction of zero-crossing	CVodeSetRootDirection	both
Disable rootfinding warnings	CVodeSetNoInactiveRootWarn	none
<b>CVDLS linear solver interface</b>		
Jacobian function	CVDlsSetJacFn	DQ
<b>CVSPILS linear solver interface</b>		
Preconditioner functions	CVSpilsSetPreconditioner	NULL, NULL
Jacobian-times-vector functions	CVSpilsSetJacTimes	NULL, DQ
Ratio between linear and nonlinear tolerances	CVSpilsSetEpsLin	0.05

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.

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.

### 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 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	<code>flag = CVodeSetErrFile(cvode_mem, errfp);</code>
Description	The function <code>CVodeSetErrFile</code> specifies a pointer to the file where all CVOICE messages should be directed when the default CVOICE error handler function is used.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block. <code>errfp</code> (FILE *) pointer to output file.
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 NULL.
Notes	The default value for <code>errfp</code> is <code>stderr</code> .  Passing a value of NULL disables all future error message output (except for the case in which the CVOICE memory pointer is NULL). This use of <code>CVodeSetErrFile</code> is strongly discouraged.   If <code>CVodeSetErrFile</code> is to be called, it should be called before any other optional input functions, in order to take effect for any later error message.

##### `CVodeSetErrHandlerFn`

Call	<code>flag = CVodeSetErrHandlerFn(cvode_mem, ehfun, eh_data);</code>
Description	The function <code>CVodeSetErrHandlerFn</code> specifies the optional user-defined function to be used in handling error messages.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block. <code>ehfun</code> (CVerHandlerFn) is the C error handler function (see §4.6.2). <code>eh_data</code> (void *) pointer to user data passed to <code>ehfun</code> every time it is called.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The function <code>ehfun</code> and data pointer <code>eh_data</code> have been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	Error messages indicating that the CVOICE solver memory is NULL will always be directed to <code>stderr</code> .

##### `CVodeSetUserData`

Call	<code>flag = CVodeSetUserData(cvode_mem, user_data);</code>
Description	The function <code>CVodeSetUserData</code> specifies the user data block <code>user_data</code> and attaches it to the main CVOICE memory block.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block. <code>user_data</code> (void *) pointer to the user data.
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 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.

#### CVodeSetMaxOrd

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

Description The function `CVodeSetMaxOrder` 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  $\leq 0$ , 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.

#### 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*).

#### 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.

**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` (booleantype) flag controlling stability limit detection (SUNTRUE = on; SUNFALSE = off).
- Return value** The return value `flag` (of type `int`) is one of  
`CV_SUCCESS` The optional value has been successfully set.  
`CV_MEM_NULL` The `cvode_mem` pointer is NULL.  
`CV_ILL_INPUT` The linear multistep method is not set to `CV_BDF`.
- Notes** The default value is `SUNFALSE`. If `stldet = SUNTRUE` when BDF is used and the method order is greater than or equal to 3, then an internal function, `CVslidet`, is called to detect a possible stability limit. If such a limit is detected, then the order is reduced.

**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  $t_0$ .

**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 ( $\geq 0.0$ ).
- 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.

**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 ( $\geq 0.0$ ).

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 **cnode\_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  $\infty$ .

#### **CNodeSetStopTime**

Call **flag** = **CNodeSetStopTime**(**cnode\_mem**, **tstop**);

Description The function **CNodeSetStopTime** specifies the value of the independent variable  $t$  past which the solution is not to proceed.

Arguments **cnode\_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 **cnode\_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.

#### **CNodeSetMaxErrTestFails**

Call **flag** = **CNodeSetMaxErrTestFails**(**cnode\_mem**, **maxnef**);

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

Arguments **cnode\_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 **cnode\_mem** pointer is **NULL**.

Notes The default value is 7.

#### **CNodeSetMaxNonlinIters**

Call **flag** = **CNodeSetMaxNonlinIters**(**cnode\_mem**, **maxcor**);

Description The function **CNodeSetMaxNonlinIters** specifies the maximum number of nonlinear solver iterations permitted per step.

Arguments **cnode\_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 **cnode\_mem** pointer or the **SUNNONLINSOL** module is **NULL**.

Notes The default value is 3.

**CVodeSetMaxConvFails**

Call	<code>flag = CVodeSetMaxConvFails(cvode_mem, maxncf);</code>
Description	The function <code>CVodeSetMaxConvFails</code> specifies the maximum number of nonlinear solver convergence failures permitted during one step.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>maxncf</code> ( <code>int</code> ) maximum number of allowable nonlinear solver convergence failures per step ( $> 0$ ).
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	The default value is 10.

**CVodeSetNonlinConvCoef**

Call	<code>flag = CVodeSetNonlinConvCoef(cvode_mem, nlscoef);</code>
Description	The function <code>CVodeSetNonlinConvCoef</code> specifies the safety factor used in the nonlinear convergence test (see §2.1).
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>nlscoef</code> ( <code>realtype</code> ) coefficient in nonlinear convergence test ( $> 0.0$ ).
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	The default value is 0.1.

**4.5.7.2 Direct linear solver interface optional input functions**

The CVDLS solver interface needs a function to compute an approximation to the Jacobian matrix  $J(t, y)$ . This function must be of type `CVDlsJacFn`. 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 CVDLS solver. To specify a user-supplied Jacobian function `jac`, CVDLS provides the function `CVDlsSetJacFn`. The CVDLS 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`.

**CVDlsSetJacFn**

Call	<code>flag = CVDlsSetJacFn(cvode_mem, jac);</code>
Description	The function <code>CVDlsSetJacFn</code> specifies the Jacobian approximation function to be used.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>jac</code> ( <code>CVDlsJacFn</code> ) user-defined Jacobian approximation function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDLS_SUCCESS</code> The optional value has been successfully set. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDLS_LMEM_NULL</code> The CVDLS linear solver interface has not been initialized.
Notes	By default, CVDLS uses an internal difference quotient function for dense and band matrices. If <code>NULL</code> is passed to <code>jac</code> , this default function is used. An error will occur if no <code>jac</code> is supplied when using a sparse matrix. The function type <code>CVDlsJacFn</code> is described in §4.6.5.

### 4.5.7.3 Iterative linear solver interface optional input functions

If preconditioning is utilized with the CVSPILS linear solver interface, then the user must supply a preconditioner solve function `psolve` and specify its name in a call to `CVSpilsSetPreconditioner`. The evaluation and preprocessing of any Jacobian-related data needed by the user's preconditioner solve function is done in the optional user-supplied function `psetup`. Both of these functions are fully specified in §4.6. If used, the `psetup` function should also be specified in the call to `CVSpilsSetPreconditioner`.

The pointer `user_data` received through `CVodeSetUserData` (or a pointer to NULL if `user_data` was not specified) is passed to the preconditioner `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.

The CVSPILS 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 CVSPILS interface. A user-defined Jacobian-vector function must be of type `CVSpilsJacTimesVecFn` and can be specified through a call to `CVSpilsSetJacTimes` (see §4.6.6 for specification details). As with the user-supplied preconditioner functions, the evaluation and processing of any Jacobian-related data needed by the user's Jacobian-times-vector function is done in the optional user-supplied function `jtsetup` (see §4.6.7 for specification details). As with the preconditioner functions, a pointer to the user-defined data structure, `user_data`, specified through `CVodeSetUserData` (or a NULL pointer otherwise) is passed to the Jacobian-times-vector setup and product functions, `jtsetup` and `jt看times`, each time they are called.

Finally, as described in Section 2.1, the CVSPILS interface requires that iterative linear solvers stop when the norm of the preconditioned residual is less than  $0.05 \cdot (0.1\epsilon)$ , where  $\epsilon$  is the nonlinear solver tolerance. The user may adjust this linear solver tolerance by calling the function `CVSpilsSetEpsLin`.

#### CVSpilsSetPreconditioner

Call	<code>flag = CVSpilsSetPreconditioner(cvode_mem, psetup, psolve);</code>
Description	The function <code>CVSpilsSetPreconditioner</code> specifies the preconditioner setup and solve functions.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>psetup</code> (CVSpilsPrecSetupFn) user-defined preconditioner setup function. Pass NULL if no setup is necessary. <code>psolve</code> (CVSpilsPrecSolveFn) user-defined preconditioner solve function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional values have been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized. <code>CVSPILS_SUNLS_FAIL</code> An error occurred when setting up preconditioning in the SUNLINSOL object used by the CVSPILS interface.
Notes	The function type <code>CVSpilsPrecSolveFn</code> is described in §4.6.8. The function type <code>CVSpilsPrecSetupFn</code> is described in §4.6.9.

#### CVSpilsSetJacTimes

Call	<code>flag = CVSpilsSetJacTimes(cvode_mem, jtsetup, jt看times);</code>
Description	The function <code>CVSpilsSetJacTimes</code> specifies the Jacobian-vector setup and product functions.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block.

	<code>jtsetup</code>	( <code>CVSpilsJacTimesSetupFn</code> ) user-defined Jacobian-vector setup function. Pass <code>NULL</code> if no setup is necessary.
	<code>jtimes</code>	( <code>CVSpilsJacTimesVecFn</code> ) user-defined Jacobian-vector product function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of	
	<code>CVSPILS_SUCCESS</code>	The optional value has been successfully set.
	<code>CVSPILS_MEM_NULL</code>	The <code>cvode_mem</code> pointer is <code>NULL</code> .
	<code>CVSPILS_LMEM_NULL</code>	The <code>CVSPILS</code> linear solver has not been initialized.
	<code>CVSPILS_SUNLS_FAIL</code>	An error occurred when setting up the system matrix-times-vector routines in the <code>SUNLINSOL</code> object used by the <code>CVSPILS</code> interface.
Notes	By default, the <code>CVSPILS</code> linear solvers use an internal difference quotient function. If <code>NULL</code> is passed to <code>jtimes</code> , this default function is used.	
	The function type <code>CVSpilsJacTimesSetupFn</code> is described in §4.6.7.	
	The function type <code>CVSpilsJacTimesVecFn</code> is described in §4.6.6.	

#### CVSpilsSetEpsLin

Call	<code>flag = CVSpilsSetEpsLin(cvode_mem, eplifac);</code>	
Description	The function <code>CVSpilsSetEpsLin</code> specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the nonlinear solver test constant.	
Arguments	<code>cvode_mem</code>	( <code>void *</code> ) pointer to the <code>CVODE</code> memory block.
	<code>eplifac</code>	( <code>realtype</code> ) linear convergence safety factor ( $\geq 0.0$ ).
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of	
	<code>CVSPILS_SUCCESS</code>	The optional value has been successfully set.
	<code>CVSPILS_MEM_NULL</code>	The <code>cvode_mem</code> pointer is <code>NULL</code> .
	<code>CVSPILS_LMEM_NULL</code>	The <code>CVSPILS</code> linear solver has not been initialized.
	<code>CVSPILS_ILL_INPUT</code>	The factor <code>eplifac</code> is negative.
Notes	The default value is 0.05.	
	If <code>eplifac= 0.0</code> is passed, the default value is used.	

#### 4.5.7.4 Rootfinding optional input functions

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

#### CVodeSetRootDirection

Call	<code>flag = CVodeSetRootDirection(cvode_mem, rootdir);</code>	
Description	The function <code>CVodeSetRootDirection</code> specifies the direction of zero-crossings to be located and returned.	
Arguments	<code>cvode_mem</code>	( <code>void *</code> ) pointer to the <code>CVODE</code> memory block.
	<code>rootdir</code>	( <code>int *</code> ) state array of length <code>nrtfn</code> , the number of root functions $g_i$ , as specified in the call to the function <code>CVodeRootInit</code> . A value of 0 for <code>rootdir[i]</code> 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 <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> .
	<code>CV_ILL_INPUT</code>	rootfinding has not been activated through a call to <code>CVodeRootInit</code> .
Notes	The default behavior is to monitor for both zero-crossing directions.	



**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 input function.

**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. <code>t</code> ( <code>realtype</code> ) the value of the independent variable at which the derivative is to be evaluated. <code>k</code> ( <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.

**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 `nniters/nsteps` measures the performance of the nonlinear solver in solving the nonlinear systems at each time step; typical values for this range from 1.1 to 1.8. The ratio `njevals/nniters` (in the case of a direct linear solver), and the ratio `npevals/nniters` (in the case of an iterative linear solver) measure the overall degree of nonlinearity in these systems, and also the quality of the approximate Jacobian or preconditioner being used. Thus, for example, `njevals/nniters` can indicate if a user-supplied Jacobian is inaccurate, if this ratio is larger than for the case of the corresponding internal Jacobian. The ratio `nliters/nniters` measures the performance of the Krylov iterative linear solver, and thus (indirectly) the quality of the preconditioner.

#### 4.5.9.1 SUNDIALS version information

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

##### **SUNDIALSGetVersion**

Call	<code>flag = SUNDIALSGetVersion(version, len);</code>
Description	The function <code>SUNDIALSGetVersion</code> fills a character array with SUNDIALS version information.
Arguments	<code>version</code> ( <code>char *</code> ) character array to hold the SUNDIALS version information. <code>len</code> ( <code>int</code> ) allocated length of the <code>version</code> character array.
Return value	If successful, <code>SUNDIALSGetVersion</code> returns 0 and <code>version</code> contains the SUNDIALS version information. Otherwise, it returns <code>-1</code> and <code>version</code> 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 <code>version</code> array are removed.

##### **SUNDIALSGetVersionNumber**

Call	<code>flag = SUNDIALSGetVersionNumber(&amp;major, &amp;minor, &amp;patch, label, len);</code>
Description	The function <code>SUNDIALSGetVersionNumber</code> set integers for the SUNDIALS major, minor, and patch release numbers and fills a character array with the release label if applicable.
Arguments	<code>major</code> ( <code>int</code> ) SUNDIALS release major version number. <code>minor</code> ( <code>int</code> ) SUNDIALS release minor version number. <code>patch</code> ( <code>int</code> ) SUNDIALS release patch version number. <code>label</code> ( <code>char *</code> ) character array to hold the SUNDIALS release label. <code>len</code> ( <code>int</code> ) allocated length of the <code>label</code> character array.
Return value	If successful, <code>SUNDIALSGetVersionNumber</code> returns 0 and the <code>major</code> , <code>minor</code> , <code>patch</code> , and <code>label</code> values are set. Otherwise, it returns <code>-1</code> 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 <code>label</code> . Any trailing characters in the <code>label</code> array are removed.

Table 4.3: Optional outputs from CVODE, CVDLS, CVDIAG, and CVSPILS

Optional output	Function name
<b>CVODE main solver</b>	
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
<b>CVDLS linear solver interface</b>	
Size of real and integer workspaces	CVDlsGetWorkSpace
No. of Jacobian evaluations	CVDlsGetNumJacEvals
No. of r.h.s. calls for finite diff. Jacobian evals.	CVDlsGetNumRhsEvals
Last return from a linear solver function	CVDlsGetLastFlag
Name of constant associated with a return flag	CVDlsGetReturnFlagName
<b>CVDIAG linear solver interface</b>	
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
<b>CVSPILS linear solver interface</b>	
Size of real and integer workspaces	CVSpilsGetWorkSpace
No. of linear iterations	CVSpilsGetNumLinIters
No. of linear convergence failures	CVSpilsGetNumConvFails
No. of preconditioner evaluations	CVSpilsGetNumPrecEvals
No. of preconditioner solves	CVSpilsGetNumPrecSolves
No. of Jacobian-vector setup evaluations	CVSpilsGetNumJTSetupEvals
No. of Jacobian-vector product evaluations	CVSpilsGetNumJtimesEvals
No. of r.h.s. calls for finite diff. Jacobian-vector evals.	CVSpilsGetNumRhsEvals
Last return from a linear solver function	CVSpilsGetLastFlag
Name of constant associated with a return flag	CVSpilsGetReturnFlagName

#### 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 `realtype` 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 `realtype` words, is given by the following:

- base value:  $\text{lenrw} = 96 + (\text{maxord}+5) * N_r + 3 * \text{nrtfn}$ ;
- using `CVodeSVtolerances`:  $\text{lenrw} = \text{lenrw} + N_r$ ;

where  $N_r$  is the number of real words in one `N_Vector` ( $\approx N$ ).

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

- base value:  $\text{leniw} = 40 + (\text{maxord}+5) * N_i + \text{nrtfn}$ ;
- using `CVodeSVtolerances`:  $\text{leniw} = \text{leniw} + N_i$ ;

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

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

- For the Adams method:  $\text{lenrw} = 96 + 17N$  and  $\text{leniw} = 57$
- For the BDF method:  $\text{lenrw} = 96 + 10N$  and  $\text{leniw} = 50$

##### 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 `cvode_mem` pointer is NULL.

**CVodeGetNumRhsEvals**

Call	<code>flag = CVodeGetNumRhsEvals(cvode_mem, &amp;nfevals);</code>
Description	The function <code>CVodeGetNumRhsEvals</code> returns the number of calls to the user's right-hand side function.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nfevals</code> (long int) number of calls to the user's <code>f</code> function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .
Notes	The <code>nfevals</code> value returned by <code>CVodeGetNumRhsEvals</code> does not account for calls made to <code>f</code> by a linear solver or preconditioner module.

**CVodeGetNumLinSolvSetups**

Call	<code>flag = CVodeGetNumLinSolvSetups(cvode_mem, &amp;nlinsetups);</code>
Description	The function <code>CVodeGetNumLinSolvSetups</code> returns the number of calls made to the linear solver's setup function.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nlinsetups</code> (long int) number of calls made to the linear solver setup function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .

**CVodeGetNumErrTestFails**

Call	<code>flag = CVodeGetNumErrTestFails(cvode_mem, &amp;netfails);</code>
Description	The function <code>CVodeGetNumErrTestFails</code> returns the number of local error test failures that have occurred.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>netfails</code> (long int) number of error test failures.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .

**CVodeGetLastOrder**

Call	<code>flag = CVodeGetLastOrder(cvode_mem, &amp;qlast);</code>
Description	The function <code>CVodeGetLastOrder</code> returns the integration method order used during the last internal step.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>qlast</code> (int) method order used on the last internal step.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .

**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.

**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.

**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.

**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.

**CVodeGetCurrentTime**

**Call** `flag = CVodeGetCurrentTime(cvode_mem, &tcure);`

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

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

**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`.

**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`.

**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`.







CV\_SUCCESS The optional output values have been successfully set.  
 CV\_MEM\_NULL The `cvode_mem` pointer or the SUNNONLINSOL module is NULL.

#### 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.

#### 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 or the SUNNONLINSOL module is NULL.

#### 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.

### 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  $i = 0, \dots, \text{nrtfn}-1$ , `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`.

#### 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.

#### 4.5.9.4 Direct linear solver interface optional output functions

The following optional outputs are available from the CVDLS modules: workspace requirements, number of calls to the Jacobian routine, number of calls to the right-hand side routine for finite-difference Jacobian approximation, and last return value from a CVDLS 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`).

#### CVDlsGetWorkSpace

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

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

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

`lenrwLS` (long int) the number of `realtype` values in the CVDLS workspace.

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

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

CVDLS\_SUCCESS The optional output values have been successfully set.

CVDLS\_MEM\_NULL The `cvode_mem` pointer is NULL.

CVDLS\_LMEM\_NULL The CVDLS 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 CVDLS is not included in this report.

#### CVDlsGetNumJacEvals

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

Description The function `CVDlsGetNumJacEvals` returns the number of calls made to the CVDLS Jacobian approximation function.

Arguments `cvode_mem` (void \*) pointer to the CVODE 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

CVDLS\_SUCCESS The optional output value has been successfully set.  
 CVDLS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
 CVDLS\_LMEM\_NULL The CVDLS linear solver has not been initialized.

#### CVDlsGetNumRhsEvals

**Call** `flag = CVDlsGetNumRhsEvals(cvode_mem, &nfevalsLS);`

**Description** The function `CVDlsGetNumRhsEvals` 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

CVDLS\_SUCCESS The optional output value has been successfully set.  
 CVDLS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
 CVDLS\_LMEM\_NULL The CVDLS linear solver has not been initialized.

**Notes** The value `nfevalsLS` is incremented only if one of the default internal difference quotient functions (dense or banded) is used.

#### CVDlsGetLastFlag

**Call** `flag = CVDlsGetLastFlag(cvode_mem, &lsflag);`

**Description** The function `CVDlsGetLastFlag` returns the last return value from a CVDLS routine.

**Arguments** `cvode_mem` (`void *`) pointer to the CVODE memory block.  
`lsflag` (`long int`) the value of the last return flag from a CVDLS function.

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

CVDLS\_SUCCESS The optional output value has been successfully set.  
 CVDLS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
 CVDLS\_LMEM\_NULL The CVDLS linear solver has not been initialized.

**Notes** If the `SUNLINSOL_DENSE` or `SUNLINSOL_BAND` setup function failed (`CVode` returned `CV_LSETUP_FAIL`), 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.

#### CVDlsGetReturnFlagName

**Call** `name = CVDlsGetReturnFlagName(lsflag);`

**Description** The function `CVDlsGetReturnFlagName` returns the name of the CVDLS constant corresponding to `lsflag`.

**Arguments** The only argument, of type `long int`, is a return flag from a CVDLS 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”.

#### 4.5.9.5 Iterative linear solver interface optional output functions

The following optional outputs are available from the CVSPILS modules: workspace requirements, 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, number of calls to the right-hand side routine for finite-difference Jacobian-vector product approximation, 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`).

##### CVSpilsGetWorkSpace

Call	<code>flag = CVSpilsGetWorkSpace(cvode_mem, &amp;lenrwLS, &amp;leniwLS);</code>
Description	The function <code>CVSpilsGetWorkSpace</code> returns the global sizes of the CVSPILS real and integer workspaces.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVMODE memory block. <code>lenrwLS</code> (long int) the number of <code>realtype</code> values in the CVSPILS workspace. <code>leniwLS</code> (long int) the number of integer values in the CVSPILS workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS.SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS.LMEM_NULL</code> The CVSPILS 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. In a parallel setting, the above values are global (i.e., summed over all processors).

##### CVSpilsGetNumLinIters

Call	<code>flag = CVSpilsGetNumLinIters(cvode_mem, &amp;nliters);</code>
Description	The function <code>CVSpilsGetNumLinIters</code> returns the cumulative number of linear iterations.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVMODE memory block. <code>nliters</code> (long int) the current number of linear iterations.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS.SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS.LMEM_NULL</code> The CVSPILS linear solver has not been initialized.

##### CVSpilsGetNumConvFails

Call	<code>flag = CVSpilsGetNumConvFails(cvode_mem, &amp;nlcfails);</code>
Description	The function <code>CVSpilsGetNumConvFails</code> returns the cumulative number of linear convergence failures.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVMODE memory block. <code>nlcfails</code> (long int) the current number of linear convergence failures.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS.SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS.LMEM_NULL</code> The CVSPILS linear solver has not been initialized.

**CVSpilsGetNumPrecEvals**

**Call**            `flag = CVSpilsGetNumPrecEvals(cvode_mem, &npevals);`

**Description**   The function `CVSpilsGetNumPrecEvals` 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

`CVSPILS_SUCCESS`    The optional output value has been successfully set.  
                  `CVSPILS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.  
                  `CVSPILS_LMEM_NULL`   The CVSPILS linear solver has not been initialized.

**CVSpilsGetNumPrecSolves**

**Call**            `flag = CVSpilsGetNumPrecSolves(cvode_mem, &npsolves);`

**Description**   The function `CVSpilsGetNumPrecSolves` 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

`CVSPILS_SUCCESS`    The optional output value has been successfully set.  
                  `CVSPILS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.  
                  `CVSPILS_LMEM_NULL`   The CVSPILS linear solver has not been initialized.

**CVSpilsGetNumJTSetupEvals**

**Call**            `flag = CVSpilsGetNumJTSetupEvals(cvode_mem, &njtsetup);`

**Description**   The function `CVSpilsGetNumJTSetupEvals` 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

`CVSPILS_SUCCESS`    The optional output value has been successfully set.  
                  `CVSPILS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.  
                  `CVSPILS_LMEM_NULL`   The CVSPILS linear solver has not been initialized.

**CVSpilsGetNumJtimesEvals**

**Call**            `flag = CVSpilsGetNumJtimesEvals(cvode_mem, &njvevals);`

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

**Arguments**    `cvode_mem` (void \*) pointer to the CVODE memory block.  
                  `njvevals` (long int) the current number of calls to `jtimes`.

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

`CVSPILS_SUCCESS`    The optional output value has been successfully set.  
                  `CVSPILS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.  
                  `CVSPILS_LMEM_NULL`   The CVSPILS linear solver has not been initialized.

**CVSpilsGetNumRhsEvals**

Call	<code>flag = CVSpilsGetNumRhsEvals(cvode_mem, &amp;nfevalsLS);</code>
Description	The function <code>CVSpilsGetNumRhsEvals</code> returns the number of calls to the user right-hand side function for finite difference Jacobian-vector product approximation.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVMODE memory block. <code>nfevalsLS</code> (long int) the number of calls to the user right-hand side function.
Return value	The return value <code>flag</code> (of type int) is one of <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.
Notes	The value <code>nfevalsLS</code> is incremented only if the default <code>CVSpilsDQJtimes</code> difference quotient function is used.

**CVSpilsGetLastFlag**

Call	<code>flag = CVSpilsGetLastFlag(cvode_mem, &amp;lsflag);</code>
Description	The function <code>CVSpilsGetLastFlag</code> returns the last return value from a CVSPILS routine.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVMODE memory block. <code>lsflag</code> (long int) the value of the last return flag from a CVSPILS function.
Return value	The return value <code>flag</code> (of type int) is one of <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.
Notes	If the CVSPILS setup function failed ( <code>CVode</code> returned <code>CV_LSETUP_FAIL</code> ), <code>lsflag</code> will be <code>SUNLS_PSET_FAIL_UNREC</code> , <code>SUNLS_ASET_FAIL_UNREC</code> , or <code>SUNLS_PACKAGE_FAIL_UNREC</code> . If the CVSPILS solve function failed ( <code>CVode</code> returned <code>CV_LSOLVE_FAIL</code> ), <code>lsflag</code> contains the error return flag from the SUNLINSOL object, which will be one of: <code>SUNLS_MEM_NULL</code> , indicating that the SUNLINSOL memory is NULL; <code>SUNLS_ATIMES_FAIL_UNREC</code> , indicating an unrecoverable failure in the $J*v$ function; <code>SUNLS_PSOLVE_FAIL_UNREC</code> , indicating that the preconditioner solve function <code>psolve</code> failed unrecoverably; <code>SUNLS_GS_FAIL</code> , indicating a failure in the Gram-Schmidt procedure (SPGMR and SPFGMR only); <code>SUNLS_QRSOL_FAIL</code> , indicating that the matrix $R$ was found to be singular during the QR solve phase (SPGMR and SPFGMR only); or <code>SUNLS_PACKAGE_FAIL_UNREC</code> , indicating an unrecoverable failure in an external iterative linear solver package.

**CVSpilsGetReturnFlagName**

Call	<code>name = CVSpilsGetReturnFlagName(lsflag);</code>
Description	The function <code>CVSpilsGetReturnFlagName</code> returns the name of the CVSPILS constant corresponding to <code>lsflag</code> .
Arguments	The only argument, of type long int, is a return flag from a CVSPILS function.
Return value	The return value is a string containing the name of the corresponding constant.

**4.5.9.6 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	<code>flag = CVDiagGetWorkSpace(cvode_mem, &amp;lenrwLS, &amp;leniwLS);</code>
Description	The function <code>CVDiagGetWorkSpace</code> returns the CVDIAG real and integer workspace sizes.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>lenrwLS</code> (long int) the number of <code>realtype</code> values in the CVDIAG workspace. <code>leniwLS</code> (long int) the number of integer values in the CVDIAG workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDIAG_SUCCESS</code> The optional output values have been successfully set. <code>CVDIAG_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDIAG_LMEM_NULL</code> 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 $3N$ <code>realtype</code> words.

**CVDiagGetNumRhsEvals**

Call	<code>flag = CVDiagGetNumRhsEvals(cvode_mem, &amp;nfevalsLS);</code>
Description	The function <code>CVDiagGetNumRhsEvals</code> returns the number of calls made to the user-supplied right-hand side function due to the finite difference Jacobian approximation.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nfevalsLS</code> (long int) the number of calls made to the user-supplied right-hand side function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDIAG_SUCCESS</code> The optional output value has been successfully set. <code>CVDIAG_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDIAG_LMEM_NULL</code> 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 <code>CVodeGetNumLinSolvSetups</code> ).

**CVDiagGetLastFlag**

Call	<code>flag = CVDiagGetLastFlag(cvode_mem, &amp;lsflag);</code>
Description	The function <code>CVDiagGetLastFlag</code> returns the last return value from a CVDIAG routine.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>lsflag</code> (long int) the value of the last return flag from a CVDIAG function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDIAG_SUCCESS</code> The optional output value has been successfully set. <code>CVDIAG_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDIAG_LMEM_NULL</code> The CVDIAG linear solver has not been initialized.
Notes	If the CVDIAG setup function failed ( <code>CVode</code> returned <code>CV_LSETUP_FAIL</code> ), the value of <code>lsflag</code> is equal to <code>CVDIAG_INV_FAIL</code> , indicating that a diagonal element with value zero was encountered. The same value is also returned if the CVDIAG solve function failed ( <code>CVode</code> returned <code>CV_LSOLVE_FAIL</code> ).

CVDiagGetReturnFlagName
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Call	<code>name = CVDiagGetReturnFlagName(lsflag);</code>
Description	The function <code>CVDiagGetReturnFlagName</code> returns the name of the CVDIAG constant corresponding to <code>lsflag</code> .
Arguments	The only argument, of type <code>long int</code> , is a return flag from a CVDIAG function.
Return value	The return value is a string containing the name of the corresponding constant.

#### 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 CVDLS or CVSPILS interface routines, as described in §4.5.3. Otherwise, all solver inputs set previously remain in effect.

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

CVodeReInit
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Call	<code>flag = CVodeReInit(cvode_mem, t0, y0);</code>
Description	The function <code>CVodeReInit</code> provides required problem specifications and reinitializes CVODE.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>t0</code> ( <code>realtype</code> ) is the initial value of $t$ . <code>y0</code> ( <code>N_Vector</code> ) is the initial value of $y$ .
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>CVodeReInit</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> Memory space for the CVODE memory block was not allocated through a previous call to <code>CVodeInit</code> . <code>CV_ILL_INPUT</code> An input argument to <code>CVodeReInit</code> has an illegal value.
Notes	If an error occurred, <code>CVodeReInit</code> also sends an error message to the error handler function.



## 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:

<b>CVRhsFn</b>	
Definition	<pre>typedef int (*CVRhsFn)(realtype t, N_Vector y, N_Vector ydot,                       void *user_data);</pre>
Purpose	This function computes the ODE right-hand side for a given value of the independent variable $t$ and state vector $y$ .
Arguments	<p><math>t</math> is the current value of the independent variable.</p> <p><math>y</math> is the current value of the dependent variable vector, <math>y(t)</math>.</p> <p><math>ydot</math> is the output vector <math>f(t, y)</math>.</p> <p><math>user\_data</math> 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 <math>y</math> 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:



**gout** is the output array, of length **nrtfn**, with components  $g_i(t, y)$ .  
**user\_data** is a pointer to user data, the same as the **user\_data** parameter passed to **CVodeSetUserData**.

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

**Notes** Allocation of memory for **gout** is automatically handled within **CVODE**.

#### 4.6.5 Jacobian information (direct method Jacobian)

If the direct linear solver interface is used (i.e., **CVDlsSetLinearSolver** is called in the steps described in §4.4), the user may provide a function of type **CVDlsJacFn** defined as follows:

**CVDlsJacFn**

**Definition**

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

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

**Arguments**

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

**Return value** A **CVDlsJacFn** should return 0 if successful, a positive value if a recoverable error occurred (in which case **CVODE** will attempt to correct, while **CVDLS** sets **last\_flag** to **CVDLS\_JACFUNC\_RECVR**), or a negative value if it failed unrecoverably (in which case the integration is halted, **CVode** returns **CV\_LSETUP\_FAIL** and **CVDLS** sets **last\_flag** to **CVDLS\_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).

Prior to calling the user-supplied Jacobian function, the Jacobian matrix  $J(t, y)$  is zeroed out, so only nonzero elements need to be loaded into **Jac**.

If the user's **CVDlsJacFn** 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 §7.1.

#### **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) = Jm,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 `realtype *col_j`, then the  $i$ -th element of the  $j$ -th column is given by `SM_COLUMN_ELEMENT_B(col_j, i, j)`, counting from 0. Thus, for  $(m, n)$  within the band,  $J_{m,n}$  can be loaded by setting `col_n = SM_COLUMN_B(J, n-1); SM_COLUMN_ELEMENT_B(col_n, m-1, n-1) = Jm,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 §7.2.

#### **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 §7.3.

### 4.6.6 Jacobian information (matrix-vector product)

If the `CVSPILS` solver interface is selected (i.e., `CVSpilsSetLinearSolver` is called in the steps described in §4.4), the user may provide a function of type `CVSpilsJacTimesVecFn` 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.

`CVSpilsJacTimesVecFn`

Definition	<pre>typedef int (*CVSpilsJacTimesVecFn)(N_Vector v, N_Vector Jv,                                      realtype t, N_Vector y, N_Vector fy,                                      void *user_data, N_Vector tmp);</pre>	
Purpose	This function computes the product $Jv = (\partial f / \partial y)v$ (or an approximation to it).	
Arguments	<b>v</b>	is the vector by which the Jacobian must be multiplied.
	<b>Jv</b>	is the output vector computed.
	<b>t</b>	is the current value of the independent variable.
	<b>y</b>	is the current value of the dependent variable vector.
	<b>fy</b>	is the current value of the vector $f(t, y)$ .
	<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to <b>CVodeSetUserData</b> .
	<b>tmp</b>	is a pointer to memory allocated for a variable of type <b>N_Vector</b> 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	<p>This function must return a value of <math>J * v</math> that uses the <i>current</i> value of <math>J</math>, i.e. as evaluated at the current <math>(t, y)</math>.</p> <p>If the user's <b>CVSpilsJacTimesVecFn</b> 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 <b>cv_mem</b> to <b>user_data</b> and then use the <b>CVodeGet*</b> functions described in §4.5.9.2. The unit roundoff can be accessed as <b>UNIT_ROUNDOFF</b> defined in <b>sundials.types.h</b>.</p>	

#### 4.6.7 Jacobian information (matrix-vector setup)

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

	<div style="border: 1px solid black; padding: 2px; display: inline-block;">CVSpilsJacTimesSetupFn</div>	
Definition	<pre>typedef int (*CVSpilsJacTimesSetupFn)(realtype t, N_Vector y,  N_Vector fy, void *user_data);</pre>	
Purpose	This function preprocesses and/or evaluates Jacobian-related data needed by the Jacobian-times-vector routine.	
Arguments	<b>t</b>	is the current value of the independent variable.
	<b>y</b>	is the current value of the dependent variable vector.
	<b>fy</b>	is the current value of the vector $f(t, y)$ .
	<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to <b>CVodeSetUserData</b> .
Return value	The value returned by the Jacobian-vector setup function should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).	
Notes	<p>Each call to the Jacobian-vector setup function is preceded by a call to the <b>CVRhsFn</b> user function with the same <math>(t, y)</math> arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.</p> <p>If the user's <b>CVSpilsJacTimesSetupFn</b> 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</p>	

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`.

#### 4.6.8 Preconditioning (linear system solution)

If preconditioning is used, then the user must provide a function to solve the linear system  $Pz = r$ , where  $P$  may be either a left or right preconditioner matrix. Here  $P$  should approximate (at least crudely) the matrix  $M = I - \gamma J$ , where  $J = \partial f / \partial y$ . If preconditioning is done on both sides, the product of the two preconditioner matrices should approximate  $M$ . This function must be of type `CVSpilsPrecSolveFn`, defined as follows:

`CVSpilsPrecSolveFn`

Definition	<pre>typedef int (*CVSpilsPrecSolveFn)(realtype t, N_Vector y, N_Vector fy,                                    N_Vector r, N_Vector z, realtype gamma,                                    realtype delta, int lr, void *user_data);</pre>	
Purpose	This function solves the preconditioned system $Pz = r$ .	
Arguments	<code>t</code>	is the current value of the independent variable.
	<code>y</code>	is the current value of the dependent variable vector.
	<code>fy</code>	is the current value of the vector $f(t, y)$ .
	<code>r</code>	is the right-hand side vector of the linear system.
	<code>z</code>	is the computed output vector.
	<code>gamma</code>	is the scalar $\gamma$ appearing in the matrix given by $M = I - \gamma J$ .
	<code>delta</code>	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 <code>delta</code> in the weighted $l_2$ norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} < \text{delta}$ . To obtain the <code>N_Vector ewt</code> , call <code>CVodeGetErrWeights</code> (see §4.5.9.2).
	<code>lr</code>	is an input flag indicating whether the preconditioner solve function is to use the left preconditioner ( <code>lr = 1</code> ) or the right preconditioner ( <code>lr = 2</code> );
	<code>user_data</code>	is a pointer to user data, the same as the <code>user_data</code> parameter passed to the function <code>CVodeSetUserData</code> .
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).	

#### 4.6.9 Preconditioning (Jacobian data)

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 `CVSpilsPrecSetupFn`, defined as follows:

`CVSpilsPrecSetupFn`

Definition	<pre>typedef int (*CVSpilsPrecSetupFn)(realtype t, N_Vector y, N_Vector fy,                                    booleantype jok, booleantype *jcurPtr,                                    realtype gamma, void *user_data);</pre>	
Purpose	This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner.	
Arguments	<code>t</code>	is the current value of the independent variable.
	<code>y</code>	is the current value of the dependent variable vector, namely the predicted value of $y(t)$ .

<b>fy</b>	is the current value of the vector $f(t, y)$ .
<b>jok</b>	is an input flag indicating whether the Jacobian-related data needs to be updated. The <b>jok</b> argument provides for the reuse of Jacobian data in the preconditioner solve function. <b>jok</b> = <b>SUNFALSE</b> means that the Jacobian-related data must be recomputed from scratch. <b>jok</b> = <b>SUNTRUE</b> means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of <b>gamma</b> ). A call with <b>jok</b> = <b>SUNTRUE</b> can only occur after a call with <b>jok</b> = <b>SUNFALSE</b> .
<b>jcurPtr</b>	is a pointer to a flag which should be set to <b>SUNTRUE</b> if Jacobian data was recomputed, or set to <b>SUNFALSE</b> if Jacobian data was not recomputed, but saved data was still reused.
<b>gamma</b>	is the scalar $\gamma$ appearing in the matrix $M = I - \gamma J$ .
<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to the function <b>CVodeSetUserData</b> .
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	<p>The operations performed by this function might include forming a crude approximate Jacobian and performing an LU factorization of the resulting approximation to <math>M = I - \gamma J</math>.</p> <p>Each call to the preconditioner setup function is preceded by a call to the <b>CVRhsFn</b> user function with the same <b>(t,y)</b> 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.</p> <p>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.</p> <p>If the user's <b>CVSpilsPrecSetupFn</b> 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 <b>cv_mem</b> to <b>user_data</b> and then use the <b>CVodeGet*</b> functions described in §4.5.9.2. The unit roundoff can be accessed as <b>UNIT_ROUNDOFF</b> defined in <b>sundials_types.h</b>.</p>

## 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 the **CVSPILS** iterative linear solver interface, in a serial setting. It uses difference quotients of the ODE right-hand side function **f** to generate a band matrix of bandwidth  $m_l + m_u + 1$ , where the number of super-diagonals ( $m_u$ , the upper half-bandwidth) and sub-diagonals ( $m_l$ , the lower half-bandwidth) are specified by the user, and uses this to form a preconditioner for use with the Krylov linear solver. Although this matrix is intended to approximate the Jacobian  $\partial f / \partial y$ , it may be a very crude approximation. The true Jacobian need not be banded, or its true bandwidth may be larger than  $m_l + m_u + 1$ , as long as the banded approximation generated here is sufficiently accurate to speed convergence as a preconditioner.

In order to use the CVBANDPRE module, the user need not define any additional functions. Aside from the header files required for the integration of the ODE problem (see §4.3), to use the CVBANDPRE module, the main program must include the header file `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

3. Set vector of initial values

4. Create CVODE object

5. Initialize CVODE solver

6. Specify integration tolerances

7. Set optional inputs

8. **Create linear solver object**

When creating the iterative linear solver object, specify the type of preconditioning (PREC\_LEFT or PREC\_RIGHT) to use.

9. Set linear solver optional inputs

10. Attach linear solver module

11. **Initialize the CVBANDPRE preconditioner module**

Specify the upper and lower half-bandwidths (`mu` and `m1`, respectively) and call

```
flag = CVBandPrecInit(cvode_mem, N, mu, m1);
```

to allocate memory and initialize the internal preconditioner data.

12. Set linear solver interface optional inputs

Note that the user should not overwrite the preconditioner setup function or solve function through calls to the `CVSpilsSetPreconditioner` optional input function.

13. Specify rootfinding problem

14. Advance solution in time

15. **Get optional outputs**

Additional optional outputs associated with CVBANDPRE are available by way of two routines described below, `CVBandPrecGetWorkspace` and `CVBandPrecGetNumRhsEvals`.

16. Deallocate memory for solution vector

17. Free solver memory

18. Free linear solver memory

The CVBANDPRE preconditioner module is initialized and attached by calling the following function:

CVBandPrecInit
----------------

Call            `flag = CVBandPrecInit(cvode_mem, N, mu, m1);`



Description	The function <code>CVBandPrecInit</code> initializes the CVBANDPRE preconditioner and allocates required (internal) memory for it.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>N</code> (sunindextype) problem dimension. <code>mu</code> (sunindextype) upper half-bandwidth of the Jacobian approximation. <code>m1</code> (sunindextype) lower half-bandwidth of the Jacobian approximation.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The call to <code>CVBandPrecInit</code> was successful. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL. <code>CVSPILS_MEM_FAIL</code> A memory allocation request has failed. <code>CVSPILS_LMEM_NULL</code> A CVSPILS linear solver memory was not attached. <code>CVSPILS_ILL_INPUT</code> 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 $-m1 \leq j - i \leq mu$ .

The following three optional output functions are available for use with the CVBANDPRE module:

#### CVBandPrecGetWorkSpace

Call	<code>flag = CVBandPrecGetWorkSpace(cvode_mem, &amp;lenrwBP, &amp;leniwBP);</code>
Description	The function <code>CVBandPrecGetWorkSpace</code> returns the sizes of the CVBANDPRE real and integer workspaces.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>lenrwBP</code> (long int) the number of <code>realtype</code> values in the CVBANDPRE workspace. <code>leniwBP</code> (long int) the number of integer values in the CVBANDPRE workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of: <code>CVSPILS_SUCCESS</code> The optional output values have been successfully set. <code>CVSPILS_PMEM_NULL</code> 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 <code>CVSpilsGetWorkSpace</code> .

#### CVBandPrecGetNumRhsEvals

Call	<code>flag = CVBandPrecGetNumRhsEvals(cvode_mem, &amp;nfevalsBP);</code>
Description	The function <code>CVBandPrecGetNumRhsEvals</code> 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	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nfevalsBP</code> (long int) the number of calls to the user right-hand side function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of: <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_PMEM_NULL</code> The CVBANDPRE preconditioner has not been initialized.
Notes	The counter <code>nfevalsBP</code> is distinct from the counter <code>nfevalsLS</code> returned by the corresponding function <code>CVSpilsGetNumRhsEvals</code> and <code>nfevals</code> returned by <code>CVodeGetNumRhsEvals</code> . The total number of right-hand side function evaluations is the sum of all three of these counters.

### 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 [28] 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 CVSPILS 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 `cfn` (of type `CVCommFn`) which performs all interprocess

communication necessary to evaluate the approximate right-hand side  $g$ . These are in addition to the user-supplied right-hand side function  $f$ . Both functions take as input the same pointer `user_data` that is passed by the user to `CVodeSetUserData` and that was passed to the user's function  $f$ . The user is responsible for providing space (presumably within `user_data`) for components of  $y$  that are communicated between processes by `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	<p><code>Nlocal</code> is the local vector length.</p> <p><code>t</code> is the value of the independent variable.</p> <p><code>y</code> is the dependent variable.</p> <p><code>glocal</code> is the output vector.</p> <p><code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code>.</p>
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	<p>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>.</p> <p>The case where <math>g</math> is mathematically identical to <math>f</math> is allowed.</p>

#### 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	<p><code>Nlocal</code> is the local vector length.</p> <p><code>t</code> is the value of the independent variable.</p> <p><code>y</code> is the dependent variable.</p> <p><code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code>.</p>
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	<p>The <code>cfm</code> function is expected to save communicated data in space defined within the data structure <code>user_data</code>.</p> <p>Each call to the <code>cfm</code> function is preceded by a call to the right-hand side function <math>f</math> with the same <math>(t, y)</math> arguments. Thus, <code>cfm</code> can omit any communication done by <math>f</math> if relevant to the evaluation of <code>glocal</code>. If all necessary communication was done in <math>f</math>, then <code>cfm</code> = <code>NULL</code> can be passed in the call to <code>CVBBDPrecInit</code> (see below).</p>

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.

- When creating the iterative linear solver object, specify the type of preconditioning (`PREC_LEFT` or `PREC_RIGHT`) to use.

- 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);
```

Note that the user should not overwrite the preconditioner setup function or solve function through calls to the `CVSpilsSetPreconditioner` optional input function.

- Additional optional outputs associated with CVBBDPRE are available by way of two routines described below, CVBBDPrecGetWorkSpace and CVBBDPrecGetNumGfnEvals.

- The user-callable functions that initialize (step 11 above) or re-initialize the CVBBDPRE preconditioner module are described next.

|             |                                                                                                                      |
|-------------|----------------------------------------------------------------------------------------------------------------------|
| Description | The function <code>CVBBDPrecInit</code> initializes and allocates (internal) memory for the CVBBDPRE preconditioner. |
|-------------|----------------------------------------------------------------------------------------------------------------------|

|           |                                                                                                                                                                                                                                                     |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Arguments | <code>cvode_mem</code> (void *) pointer to the CVODE memory block.                                                                                                                                                                                  |
|           | <code>local_N</code> (sunindextype) local vector length.                                                                                                                                                                                            |
|           | <code>mudq</code> (sunindextype) upper half-bandwidth to be used in the difference quotient Jacobian approximation.                                                                                                                                 |
|           | <code>mldq</code> (sunindextype) lower half-bandwidth to be used in the difference quotient Jacobian approximation.                                                                                                                                 |
|           | <code>mukeep</code> (sunindextype) upper half-bandwidth of the retained banded approximate Jacobian block.                                                                                                                                          |
|           | <code>mlkeep</code> (sunindextype) lower half-bandwidth of the retained banded approximate Jacobian block.                                                                                                                                          |
|           | <code>dqrely</code> (realtype) the relative increment in components of $y$ used in the difference quotient approximations. The default is $\text{dqrely} = \sqrt{\text{unit roundoff}}$ , which can be specified by passing $\text{dqrely} = 0.0$ . |
|           | <code>gloc</code> (CVLocalFn) the C function which computes the approximation $g(t, y) \approx f(t, y)$ .                                                                                                                                           |
|           | <code>cfn</code> (CVCommFn) the optional C function which performs all interprocess communication required for the computation of $g(t, y)$ .                                                                                                       |

|              |                                                                                                                      |
|--------------|----------------------------------------------------------------------------------------------------------------------|
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of                                             |
|              | <code>CVSPILS_SUCCESS</code> The call to <code>CVBBDPrecInit</code> was successful.                                  |
|              | <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.                                           |
|              | <code>CVSPILS_MEM_FAIL</code> A memory allocation request has failed.                                                |
|              | <code>CVSPILS_LMEM_NULL</code> A CVSPILS linear solver was not attached.                                             |
|              | <code>CVSPILS_ILL_INPUT</code> 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.

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 `CVSpilsSet***` functions, must also be made (in the proper order).

#### CVBBDPrecReInit

|             |                                                                                                                     |
|-------------|---------------------------------------------------------------------------------------------------------------------|
| Call        | <code>flag = CVBBDPrecReInit(cvode_mem, mudq, mldq, dqrely);</code>                                                 |
| Description | The function <code>CVBBDPrecReInit</code> re-initializes the CVBBDPRE preconditioner.                               |
| Arguments   | <code>cvode_mem</code> (void *) pointer to the CVODE memory block.                                                  |
|             | <code>mudq</code> (sunindextype) upper half-bandwidth to be used in the difference quotient Jacobian approximation. |

**mldq** (sunindextype) lower half-bandwidth to be used in the difference quotient Jacobian approximation.

**dqrely** (realtype) the relative increment in components of **y** used in the difference quotient approximations. The default is  $\text{dqrely} = \sqrt{\text{unit roundoff}}$ , which can be specified by passing  $\text{dqrely} = 0.0$ .

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

**CVSPILS\_SUCCESS** The call to **CVBBDPrecReInit** was successful.

**CVSPILS\_MEM\_NULL** The **cvode\_mem** pointer was **NULL**.

**CVSPILS\_LMEM\_NULL** A **CVSPILS** linear solver memory was not attached.

**CVSPILS\_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.

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 **realtype** values in the **CVBBDPRE** workspace.

**leniwBBDP** (long int) local number of integer values in the **CVBBDPRE** workspace.

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

**CVSPILS\_SUCCESS** The optional output value has been successfully set.

**CVSPILS\_MEM\_NULL** The **cvode\_mem** pointer was **NULL**.

**CVSPILS\_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 **CVSpilsGetWorkSpace**.

#### CVBBDPrecGetNumGfnEvals

**Call** `flag = CVBBDPrecGetNumGfnEvals(cvode_mem, &ngevalsBBDP);`

**Description** The function **CVBBDPrecGetNumGfnEvals** returns the number of calls made to the user-supplied **gloc** function due to the finite difference approximation of the Jacobian blocks used within the preconditioner setup function.

**Arguments** **cvode\_mem** (void \*) pointer to the **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

**CVSPILS\_SUCCESS** The optional output value has been successfully set.

**CVSPILS\_MEM\_NULL** The **cvode\_mem** pointer was **NULL**.

**CVSPILS\_PMEM\_NULL** The **CVBBDPRE** preconditioner has not been initialized.

In addition to the **ngevalsBBDP** **gloc** evaluations, the costs associated with **CVBBDPRE** also include **nlinsetups** LU factorizations, **nlinsetups** calls to **cfm**, **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

# FCVODE, an Interface Module for FORTRAN Applications

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

### 5.1 Important note on portability

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

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

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

### 5.2 Fortran Data Types

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

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

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

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

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

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

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

### 5.3 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 `SUNBandLinearSolver`.
  - `FSUNDENSELINSOLINIT` (defined by `SUNLINSOL_DENSE`) interfaces to `SUNDenseLinearSolver`.
  - `FSUNKLUINIT` (defined by `SUNLINSOL_KLU`) interfaces to `SUNKLU`.
  - `FSUNKLUREINIT` (defined by `SUNLINSOL_KLU`) interfaces to `SUNKLUREinit`.
  - `FSUNLAPACKBANDINIT` (defined by `SUNLINSOL_LAPACKBAND`) interfaces to `SUNLapackBand`.
  - `FSUNLAPACKDENSEINIT` (defined by `SUNLINSOL_LAPACKDENSE`) interfaces to `SUNLapackDense`.
  - `FSUNPCGINIT` (defined by `SUNLINSOL_PCG`) interfaces to `SUNPCG`.
  - `FSUNSPBCGSINIT` (defined by `SUNLINSOL_SPBCGS`) interfaces to `SUNSPBCGS`.
  - `FSUNSPFGMRINIT` (defined by `SUNLINSOL_SPFGMR`) interfaces to `SUNSPFGMR`.
  - `FSUNSPGMRINIT` (defined by `SUNLINSOL_SPGMR`) interfaces to `SUNSPGMR`.
  - `FSUNSPTFQMRINIT` (defined by `SUNLINSOL_SPTFQMR`) interfaces to `SUNSPTFQMR`.
  - `FSUNSUPERLUMTINIT` (defined by `SUNLINSOL_SUPERLUMT`) interfaces to `SUNSuperLUMT`.
- Interface to the main CVODE module
  - `FCVMALLOC` interfaces to `CVodeCreate`, `CVodeSetUserData`, and `CVodeInit`, as well as one of `CVodeSStolerances` or `CVodeSVtolerances`.



- FCVREINIT interfaces to CNodeReInit.
- FCVSETIIN and FCVSETRIN interface to CNodeSet\* functions.
- FCVEWTSET interfaces to CNodeWftolerances.
- FCVODE interfaces to CNode, CNodeGet\* functions, and to the optional output functions for the selected linear solver module.
- FCVDKY interfaces to the interpolated output function CNodeGetDky.
- FCVGETERWEIGHTS interfaces to CNodeGetErrWeights.
- FCVGTESTLOCALERR interfaces to CNodeGetEstLocalErrors.
- FCVFREE interfaces to CNodeFree.
- Interface to the linear solver interfaces
  - FCVDLSINIT interfaces to CVDlsSetLinearSolver.
  - FCVDENSESETJAC interfaces to CVDlsSetJacFn.
  - FCVBANDSETJAC interfaces to CVDlsSetJacFn.
  - FCVSPARSESETJAC interfaces to CVDlsSetJacFn.
  - FCVSPILSINIT interfaces to CVSpilsSetLinearSolver.
  - FCVSPILSSETEPSLIN interfaces to CVSpilsSetEpsLin.
  - FCVSPILSSETJAC interfaces to CVSpilsSetJacTimes.
  - FCVSPILSSETPREC interfaces to CVSpilsSetPreconditioner.
  - FCVDIAG interfaces to CVDiag.
- Interface to the nonlinear solver interface
  - FCVNLSINIT interfaces to CVSetNonlinearSolver.

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

| FCVODE routine<br>(FORTRAN, user-supplied) | CVOICE function<br>(C, interface) | CVOICE type of<br>interface function |
|--------------------------------------------|-----------------------------------|--------------------------------------|
| FCVFUN                                     | FCVf                              | CVRhsFn                              |
| FCVEWT                                     | FCVEwtSet                         | CVEwtFn                              |
| FCVDJAC                                    | FCVDenseJac                       | CVDlsJacFn                           |
| FCVBjac                                    | FCVBandJac                        | CVDlsJacFn                           |
| FCVSPJAC                                   | FCVSparsJac                       | CVDlsJacFn                           |
| FCVPSOL                                    | FCVPSol                           | CVSpilsPrecSolveFn                   |
| FCVPSET                                    | FCVPSet                           | CVSpilsPrecSetupFn                   |
| FCVJTtimes                                 | FCVJtimes                         | CVSpilsJacTimesVecFn                 |
| FCVJTSETUP                                 | FCVJTSetup                        | CVSpilsJacTimesSetupFn               |

In contrast to the case of direct use of CVOICE, 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.

## 5.4 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 CVOICE 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 FCFUN(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 FCFMALLOC. 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 §9.2). 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 §9.3.

#### 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,<br>& 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>T0 is the initial value of <math>t</math>.</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 5.2.

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

## 7. Set optional inputs

Call `FCVINSETIIN` and/or `FCVINSETRIN` to set desired optional inputs, if any. See §5.5 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 `FCVODE` must initialize the `CVDLS` or `CVSPILS` linear solver interface.

### CVDLS direct linear solver interface

To attach a direct `SUNLINSOL` object and corresponding `SUNMATRIX` object to the `CVDLS` interface, then following calls to initialize the `SUNLINSOL` and `SUNMATRIX` objects in steps 3 and 4 above, the user must make the call:

```
CALL FCVDLSINIT(IER)
```

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

Optional outputs specific to the `CVDLS` case are listed in Table 5.2.

**CVDLS with dense Jacobian matrix** As an option when using the `CVDLS` interface with `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 `FCVDLSINIT`, 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.

**CVDLS with band Jacobian matrix** As an option when using the CVDLS interface with `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  $k = i - j + \text{MU} + 1$  ( $k = 1 \cdots \text{ML} + \text{MU} + 1$ ) 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 `FCVDLSINIT`, 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.

**CVDLS with sparse Jacobian matrix** When using the CVDLS interface with SUNLINSOL\_KLU or SUNLINSOL\_SUPERLUMT linear solvers, the user must supply the **FCVSPJAC** routine that computes a compressed-sparse-column or compressed-sparse-row if using KLU 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 **sunmatrix\_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 **FCVDLSINIT**, 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.

#### CVSPILS iterative linear solver interface

To attach an iterative SUNLINSOL object to the CVSPILS interface, then following the call to initialize the SUNLINSOL object in step 4 above, the user must make the call:

```
CALL FCVSPILSINIT(IER)
```

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

Optional outputs specific to the CVSPILS case are listed in Table 5.2.

#### Functions used by CVSPILS

Optional user-supplied routines **FCVJTIMES** and **FCVJTSETUP** (see below), can be provided for Jacobian-vector products. If they are, then, following the call to **FCVSPILSINIT**, the user must make the call:

```
CALL FCVSPILSSETJAC(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.

If preconditioning is to be done, then the user must call

```
CALL FCVSPILSSETPREC(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** (see below).

**User-supplied routines for CVSPILS**

With treatment of the linear systems by any of the Krylov iterative solvers, there are four optional user-supplied routines — FCVJTIMES, FCVJTSETUP, FCVPSOL, and FCVPSET. The specifications for these routines are given below.

As an option when using the CVSPILS 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.

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



If preconditioning is to be included, 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.



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

### Notes

- (a) If the user's FCVJTIMES or 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  $\ell_2$  norm, i.e.  $\sqrt{\sum (\rho_i * EWT[i])^2} < DELTA$ .
- (b) If needed in FCVJTIMES, FCVJTSETUP, 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 FCVJTIMES, FCVJTSETUP, 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 5.2.

## 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 5.2).

### 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 `FCVMALLOC`. `FCVREINIT` performs the same initializations as `FCVMALLOC`, but does no memory allocation, using instead the existing internal memory created by the previous `FCVMALLOC` 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 `CVDLS` or `CVSPILS` interface, as shown above. If only linear solver parameters are being modified, then these calls may be made without re-attaching to the `CVDLS` or `CVSPILS` interface.

### 13. Memory deallocation

To free the internal memory created by the call to `FCVMALLOC`, `FCVDLSINIT`/`FCVSPILSINIT`, `FNVINIT*` and `FSUN***MATINIT`, make the call

```
CALL FCVFREE
```

## 5.5 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 two routines: `FCVSETIIN` for integer optional inputs and `FCVSETRIN` for real optional inputs. These functions should be called as follows:

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

Table 5.1: 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 $t_{\text{out}}$ | 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_WARN                           | 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                    | $\infty$      |
| MIN_STEP                         | Minimum absolute step size                    | 0.0           |
| STOP_TIME                        | Value of $t_{\text{stop}}$                    | undefined     |
| NLCONV_COEF                      | Coefficient in the nonlinear convergence test | 0.1           |

where **KEY** is a quoted string indicating which optional input is set (see Table 5.1), **IVAL** is the integer input value to be used, **RVAL** is the real input value 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`.

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 **FCVMALOC**. Table 5.2 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)
```

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.

## 5.6 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:

Table 5.2: 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              |
| CVDLS linear solver interface   |                 |                                |
| 13                              | LENRWLS         | CVDlsGetWorkSpace              |
| 14                              | LENIWLS         | CVDlsGetWorkSpace              |
| 15                              | LS_FLAG         | CVDlsGetLastFlag               |
| 16                              | NFELS           | CVDlsGetNumRhsEvals            |
| 17                              | NJE             | CVDlsGetNumJacEvals            |
| CVSPILS linear solver interface |                 |                                |
| 13                              | LENRWLS         | CVSpilsGetWorkSpace            |
| 14                              | LENIWLS         | CVSpilsGetWorkSpace            |
| 15                              | LS_FLAG         | CVSpilsGetLastFlag             |
| 16                              | NFELS           | CVSpilsGetNumRhsEvals          |
| 17                              | NJTV            | CVSpilsGetNumJacEvals          |
| 18                              | NPE             | CVSpilsGetNumPrecEvals         |
| 19                              | NPS             | CVSpilsGetNumPrecSolves        |
| 20                              | NLI             | CVSpilsGetNumLinIters          |
| 21                              | NCFL            | CVSpilsGetNumConvFails         |
| CVDIAG linear solver interface  |                 |                                |
| 13                              | LENRWLS         | CVDdiagGetWorkSpace            |
| 14                              | LENIWLS         | CVDdiagGetWorkSpace            |
| 15                              | LS_FLAG         | CVDdiagGetLastFlag             |
| 16                              | NFELS           | CVDdiagGetNumRhsEvals          |

| 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          |

- 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)` ( $i = 1, \dots, \text{NRTFN}$ ) are 0 or  $\pm 1$ , 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
```

## 5.7 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 `CVODE` 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 `CVSPILS` interface and any of the Krylov iterative linear solvers.

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

- `FCVBPINIT` interfaces to `CVBandPrecInit`.
- `FCVBPOPT` 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 §5.4 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. **Problem specification**

5. **Set optional inputs**

6. **Linear solver interface specification**

First, initialize the CVSPILS iterative linear solver interface by calling `FCVSPILSINIT`.

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 CVSPILS should use the supplied `FCVJTIMES` and `FCVJTSETUP`, make the call

```
CALL FCVSPILSSETJAC(FLAG, IER)
```

with `FLAG`  $\neq 0$  (see step 8 in §5.4 for details).

7. **Problem solution**

8. **Additional solution output**

9. **CVBANDPRE Optional outputs**

Optional outputs specific to the CVSPILS solver interface are listed in Table 5.2. 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.

10. **Memory deallocation**

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

## 5.8 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 FCFUN, 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<br>(FORTRAN, user-supplied) | CVODE function<br>(C, interface) | CVODE type of<br>interface function |
|--------------------------------------------|----------------------------------|-------------------------------------|
| FCVLOCfN                                   | FCVgloc                          | CVLocalFn                           |
| FCVCOMMF                                   | FCVcfn                           | CVCommFn                            |
| FCVJTfN                                    | FCVJtimes                        | CVSpilsJacTimesVecFn                |
| FCVJTSETUP                                 | FCVJTSetup                       | CVSpilsJacTimesSetupFn              |

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 §5.3, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fcvbdd.h`.

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

1. **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. **Problem specification**
5. **Set optional inputs**
6. **Linear solver interface specification**

First, initialize the CVSPILS iterative linear solver interface by calling FCVSPILSINIT.

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 FCVSPILSSETJAC(FLAG, IER)
```

with  $\text{FLAG} \neq 0$  (see step 8 in §5.4 for details).

## 7. Problem solution

## 8. Additional solution output

## 9. CVBBDPRE Optional outputs

Optional outputs specific to the CVSPILS solver interface are listed in Table 5.2. To obtain the optional outputs associated with the CVBBDPRE module, make the following call:

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

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. NGEBBBD is the number of  $g(t, y)$  evaluations (calls to FCVLOCFN) so far.

## 10. 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 FCVSPILSINIT must also be made; in this case the linear solver memory is reallocated.

## 11. Memory deallocation

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

## 12. 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 §5.4.



## Chapter 6

# Description of the NVECTOR module

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

The generic `N_Vector` type is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the vector, and an *ops* field pointing to a structure with generic vector operations. The type `N_Vector` is defined as

```
typedef struct _generic_N_Vector *N_Vector;
```

```
struct _generic_N_Vector {  
    void *content;  
    struct _generic_N_Vector_Ops *ops;  
};
```

The `_generic_N_Vector_Ops` structure is essentially a list of pointers to the various actual vector operations, and is defined as

```
struct _generic_N_Vector_Ops {  
    N_Vector_ID (*nvgetvectorid)(N_Vector);  
    N_Vector (*nvclone)(N_Vector);  
    N_Vector (*nvcloneempty)(N_Vector);  
    void (*nvdestroy)(N_Vector);  
    void (*nvspace)(N_Vector, sunindextype *, sunindextype *);  
    realtype* (*nvgetarraypointer)(N_Vector);  
    void (*nvsetarraypointer)(realtype *, N_Vector);  
    void (*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    (*nvlinorm)(N_Vector);
void        (*nvcompare)(realtype, N_Vector, N_Vector);
boolean_t   (*nvinvtest)(N_Vector, N_Vector);
boolean_t   (*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*);
};

```

The generic NVECTOR module defines and implements the vector operations acting on an `N_Vector`. These routines are nothing but wrappers for the vector operations defined by a particular NVECTOR implementation, which are accessed through the `ops` field of the `N_Vector` structure. To illustrate this point we show below the implementation of a typical vector operation from the generic NVECTOR module, namely `N_VScale`, which performs the scaling of a vector `x` by a scalar `c`:

```

void N_VScale(realtype c, N_Vector x, N_Vector z)
{
    z->ops->nvscale(c, x, z);
}

```

Table 6.2 contains a complete list of all standard vector operations defined by the generic NVECTOR module. Tables 6.3 and 6.4 list *optional* fused and vector array operations respectively. These 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 one of the fused or vector array operations as `NULL`, the NVECTOR interface will call one of the standard vector operations as necessary.

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

```

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

```

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

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

```

void N_VDestroyVectorArray(N_Vector *vs, int count);

```

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

A particular implementation of the NVECTOR module must:

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_CUSTOM   | User-provided custom vector         | 6        |

- Specify the *content* field of `N_Vector`.
- Define and implement the vector operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one NVECTOR module (each with different `N_Vector` internal data representations) in the same code.
- Define and implement user-callable constructor and destructor routines to create and free an `N_Vector` with the new *content* field and with *ops* pointing to the new vector operations.
- Optionally, define and implement additional user-callable routines acting on the newly defined `N_Vector` (e.g., a routine to print the content for debugging purposes).
- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the *content* field of the newly defined `N_Vector`.

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

Table 6.2: Description of the NVECTOR operations

| Name                          | Usage and Description                                                                                                                                                                                                                                                                        |
|-------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>N_VGetVectorID</code>   | <code>id = N_VGetVectorID(w);</code><br>Returns the vector type identifier for the vector <code>w</code> . It is used to determine the vector implementation type (e.g. serial, parallel, . . . ) from the abstract <code>N_Vector</code> interface. Returned values are given in Table 6.1. |
| <code>N_VClone</code>         | <code>v = N_VClone(w);</code><br>Creates a new <code>N_Vector</code> of the same type as an existing vector <code>w</code> and sets the <i>ops</i> field. It does not copy the vector, but rather allocates storage for the new vector.                                                      |
| <i>continued on next page</i> |                                                                                                                                                                                                                                                                                              |

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|---------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                            | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| N_VCloneEmpty                   | <code>v = N_VCloneEmpty(w);</code><br>Creates a new <b>N_Vector</b> of the same type as an existing vector <b>w</b> and sets the <i>ops</i> field. It does not allocate storage for data.                                                                                                                                                                                                                                                                                                                                                |
| N_VDestroy                      | <code>N_VDestroy(v);</code><br>Destroys the <b>N_Vector</b> <b>v</b> and frees memory allocated for its internal data.                                                                                                                                                                                                                                                                                                                                                                                                                   |
| N_VSpace                        | <code>N_VSpace(nvSpec, &amp;lrw, &amp;liw);</code><br>Returns storage requirements for one <b>N_Vector</b> . <b>lrw</b> contains the number of realtype words and <b>liw</b> 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.                                                                                                                      |
| N_VGetArrayPointer              | <code>vdata = N_VGetArrayPointer(v);</code><br>Returns a pointer to a <b>realtype</b> array from the <b>N_Vector</b> <b>v</b> . Note that this assumes that the internal data in <b>N_Vector</b> is a contiguous array of <b>realtype</b> . This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, the sparse linear solvers (serial and threaded), and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS. |
| N_VSetArrayPointer              | <code>N_VSetArrayPointer(vdata, v);</code><br>Overwrites the data in an <b>N_Vector</b> with a given array of <b>realtype</b> . Note that this assumes that the internal data in <b>N_Vector</b> is a contiguous array of <b>realtype</b> . This routine is only used in the interfaces to the dense (serial) linear solver, hence need not exist in a user-supplied NVECTOR module for a parallel environment.                                                                                                                          |
| N_VLinearSum                    | <code>N_VLinearSum(a, x, b, y, z);</code><br>Performs the operation $z = ax + by$ , where <i>a</i> and <i>b</i> are <b>realtype</b> scalars and <i>x</i> and <i>y</i> are of type <b>N_Vector</b> : $z_i = ax_i + by_i$ , $i = 0, \dots, n-1$ .                                                                                                                                                                                                                                                                                          |
| N_VConst                        | <code>N_VConst(c, z);</code><br>Sets all components of the <b>N_Vector</b> <b>z</b> to <b>realtype</b> <i>c</i> : $z_i = c$ , $i = 0, \dots, n-1$ .                                                                                                                                                                                                                                                                                                                                                                                      |
| N_VProd                         | <code>N_VProd(x, y, z);</code><br>Sets the <b>N_Vector</b> <b>z</b> to be the component-wise product of the <b>N_Vector</b> inputs <b>x</b> and <b>y</b> : $z_i = x_i y_i$ , $i = 0, \dots, n-1$ .                                                                                                                                                                                                                                                                                                                                       |
| <i>continued on next page</i>   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |

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|---------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                            | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| N_VDiv                          | <p><b>N_VDiv(x, y, z);</b><br/> Sets the <b>N_Vector</b> <b>z</b> to be the component-wise ratio of the <b>N_Vector</b> inputs <b>x</b> and <b>y</b>: <math>z_i = x_i/y_i</math>, <math>i = 0, \dots, n-1</math>. The <math>y_i</math> may not be tested for 0 values. It should only be called with a <b>y</b> that is guaranteed to have all nonzero components.</p>                                                                                                               |
| N_VScale                        | <p><b>N_VScale(c, x, z);</b><br/> Scales the <b>N_Vector</b> <b>x</b> by the <b>realtype</b> scalar <b>c</b> and returns the result in <b>z</b>: <math>z_i = cx_i</math>, <math>i = 0, \dots, n-1</math>.</p>                                                                                                                                                                                                                                                                        |
| N_VAbs                          | <p><b>N_VAbs(x, z);</b><br/> Sets the components of the <b>N_Vector</b> <b>z</b> to be the absolute values of the components of the <b>N_Vector</b> <b>x</b>: <math>y_i =  x_i </math>, <math>i = 0, \dots, n-1</math>.</p>                                                                                                                                                                                                                                                          |
| N_VInv                          | <p><b>N_VInv(x, z);</b><br/> Sets the components of the <b>N_Vector</b> <b>z</b> to be the inverses of the components of the <b>N_Vector</b> <b>x</b>: <math>z_i = 1.0/x_i</math>, <math>i = 0, \dots, n-1</math>. This routine may not check for division by 0. It should be called only with an <b>x</b> which is guaranteed to have all nonzero components.</p>                                                                                                                   |
| N_VAddConst                     | <p><b>N_VAddConst(x, b, z);</b><br/> Adds the <b>realtype</b> scalar <b>b</b> to all components of <b>x</b> and returns the result in the <b>N_Vector</b> <b>z</b>: <math>z_i = x_i + b</math>, <math>i = 0, \dots, n-1</math>.</p>                                                                                                                                                                                                                                                  |
| N_VDotProd                      | <p><b>d = N_VDotProd(x, y);</b><br/> Returns the value of the ordinary dot product of <b>x</b> and <b>y</b>: <math>d = \sum_{i=0}^{n-1} x_i y_i</math>.</p>                                                                                                                                                                                                                                                                                                                          |
| N_VMaxNorm                      | <p><b>m = N_VMaxNorm(x);</b><br/> Returns the maximum norm of the <b>N_Vector</b> <b>x</b>: <math>m = \max_i  x_i </math>.</p>                                                                                                                                                                                                                                                                                                                                                       |
| N_VWrmsNorm                     | <p><b>m = N_VWrmsNorm(x, w)</b><br/> Returns the weighted root-mean-square norm of the <b>N_Vector</b> <b>x</b> with <b>realtype</b> weight vector <b>w</b>: <math>m = \sqrt{(\sum_{i=0}^{n-1} (x_i w_i)^2) / n}</math>.</p>                                                                                                                                                                                                                                                         |
| N_VWrmsNormMask                 | <p><b>m = N_VWrmsNormMask(x, w, id);</b><br/> Returns the weighted root mean square norm of the <b>N_Vector</b> <b>x</b> with <b>realtype</b> weight vector <b>w</b> built using only the elements of <b>x</b> corresponding to positive elements of the <b>N_Vector</b> <b>id</b>:<br/> <math display="block">m = \sqrt{(\sum_{i=0}^{n-1} (x_i w_i H(id_i))^2) / n}, \text{ where } H(\alpha) = \begin{cases} 1 &amp; \alpha &gt; 0 \\ 0 &amp; \alpha \leq 0 \end{cases}</math></p> |
| <i>continued on next page</i>   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

| <i>continued from last page</i> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|---------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                            | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| N_VMin                          | <code>m = N_VMin(x);</code><br>Returns the smallest element of the N_Vector <code>x</code> : $m = \min_i x_i$ .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
| N_VWL2Norm                      | <code>m = N_VWL2Norm(x, w);</code><br>Returns the weighted Euclidean $\ell_2$ norm of the N_Vector <code>x</code> with <code>realtype</code> weight vector <code>w</code> : $m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}$ .                                                                                                                                                                                                                                                                                                                                                                                   |
| N_VL1Norm                       | <code>m = N_VL1Norm(x);</code><br>Returns the $\ell_1$ norm of the N_Vector <code>x</code> : $m = \sum_{i=0}^{n-1}  x_i $ .                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| N_VCompare                      | <code>N_VCompare(c, x, z);</code><br>Compares the components of the N_Vector <code>x</code> to the <code>realtype</code> scalar <code>c</code> and returns an N_Vector <code>z</code> such that: $z_i = 1.0$ if $ x_i  \geq c$ and $z_i = 0.0$ otherwise.                                                                                                                                                                                                                                                                                                                                                 |
| N_VInvTest                      | <code>t = N_VInvTest(x, z);</code><br>Sets the components of the N_Vector <code>z</code> to be the inverses of the components of the N_Vector <code>x</code> , with prior testing for zero values: $z_i = 1.0/x_i$ , $i = 0, \dots, n-1$ . This routine returns a boolean assigned to <code>SUNTRUE</code> if all components of <code>x</code> are nonzero (successful inversion) and returns <code>SUNFALSE</code> otherwise.                                                                                                                                                                            |
| N_VConstrMask                   | <code>t = N_VConstrMask(c, x, m);</code><br>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 <code>SUNFALSE</code> if any element failed the constraint test and assigned to <code>SUNTRUE</code> if all passed. It also sets a mask vector <code>m</code> , with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking. |
| N_VMinQuotient                  | <code>minq = N_VMinQuotient(num, denom);</code><br>This routine returns the minimum of the quotients obtained by term-wise dividing <code>num<sub>i</sub></code> by <code>denom<sub>i</sub></code> . A zero element in <code>denom</code> will be skipped. If no such quotients are found, then the large value <code>BIG_REAL</code> (defined in the header file <code>sundials.types.h</code> ) is returned.                                                                                                                                                                                            |

Table 6.3: Description of the NVECTOR fused operations

*continued on next page*

| <i>continued from last page</i> |                       |
|---------------------------------|-----------------------|
| Name                            | Usage and Description |

Table 6.4: Description of the NVECTOR vector array operations

| Name                          | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
|-------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| N_VLinearSumVectorArray       | <p><code>ier = N_VLinearSumVectorArray(nv, a, X, b, Y, Z);</code><br/> This routine computes the linear sum of two vector arrays containing <math>nv</math> vectors of <math>n</math> elements:</p> $z_{j,i} = ax_{j,i} + by_{j,i}, \quad i = 1, \dots, n \quad j = 1, \dots, nv,$ <p>where <math>a</math> and <math>b</math> are <b>realtype</b> scalars and <math>X</math>, <math>Y</math>, and <math>Z</math> are arrays of <math>nv</math> vectors (type <b>N_Vector*</b>). The operation returns 0 for success and a non-zero value otherwise.</p>  |
| N_VScaleVectorArray           | <p><code>ier = N_VScaleVectorArray(nv, c, X, Z);</code><br/> This routine scales each vector of <math>n</math> elements in a vector array of <math>nv</math> vectors by a potentially different constant:</p> $z_{j,i} = c_j x_{j,i}, \quad i = 1, \dots, n \quad j = 1, \dots, nv,$ <p>where <math>c</math> is an array of <math>nv</math> scalars (type <b>realtype*</b>) and <math>X</math> and <math>Z</math> are arrays of <math>nv</math> vectors (type <b>N_Vector*</b>). The operation returns 0 for success and a non-zero value otherwise.</p> |
| N_VConstVectorArray           | <p><code>ier = N_VConstVectorArray(nv, c, X);</code><br/> This routine sets each element in a vector of <math>n</math> elements in a vector array of <math>nv</math> vectors to the same value:</p> $z_{j,i} = c, \quad i = 1, \dots, n \quad j = 1, \dots, nv,$ <p>where <math>c</math> is a <b>realtype</b> scalar and <math>X</math> is an array of <math>nv</math> vectors (type <b>N_Vector*</b>). The operation returns 0 for success and a non-zero value otherwise.</p>                                                                          |
| <i>continued on next page</i> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |



| continued from last page    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|-----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                        | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| N_VWrmsNormVectorArray      | <p><code>ier = N_VWrmsNormVectorArray(nv, X, W, m);</code><br/> This routine computes the weighted root mean square norm of <math>nv</math> vectors with <math>n</math> elements:</p> $m_j = \left( \frac{1}{n} \sum_{i=1}^n (x_{j,i} w_{j,i})^2 \right)^{1/2}, \quad j = 1, \dots, nvec,$ <p>where <math>m</math> (type <code>realtype*</code>) contains the <math>nv</math> norms of the vectors in the vector array <math>X</math> (type <code>N_Vector*</code>) with corresponding weight vectors <math>W</math> (type <code>N_Vector*</code>). The operation returns 0 for success and a non-zero value otherwise.</p>                                                                                                                                                                                                                                                |
| N_VWrmsNormMaskVectorArray  | <p><code>ier = N_VWrmsNormMaskVectorArray(nv, X, W, id, m);</code><br/> This routine computes the masked weighted root mean square norm of <math>nv</math> vectors with <math>n</math> elements:</p> $m_j = \left( \frac{1}{n} \sum_{i=1}^n (x_{j,i} w_{j,i} H(id_i))^2 \right)^{1/2}, \quad j = 1, \dots, nvec,$ <p><math>H(id_i) = 1</math> for <math>id_i &gt; 0</math> and is zero otherwise, <math>m</math> (type <code>realtype*</code>) contains the <math>nv</math> norms of the vectors in the vector array <math>X</math> (type <code>N_Vector*</code>) with corresponding weight vectors <math>W</math> (type <code>N_Vector*</code>) and mask vector <math>id</math> (type <code>N_Vector</code>). The operation returns 0 for success and a non-zero value otherwise.</p>                                                                                     |
| N_VScaleAddMultiVectorArray | <p><code>ier = N_VScaleAddMultiVectorArray(nv, ns, c, X, YY, ZZ);</code><br/> This routine scales and adds a vector in a vector array of <math>nv</math> vectors to the corresponding vector in <math>ns</math> vector arrays:</p> $z_{j,i} = \sum_{k=1}^{ns} c_k x_{k,j,i}, \quad i = 1, \dots, n \quad j = 1, \dots, nv,$ <p>where <math>c</math> is an array of <math>ns</math> scalars (type <code>realtype*</code>), <math>X</math> is a vector array of <math>nv</math> vectors (type <code>idN_Vector*</code>) to be scaled and added to the corresponding vector in each of the <math>ns</math> vector arrays in the array of vector arrays <math>YY</math> (type <code>N_Vector**</code>) and stored in the output array of vector arrays <math>ZZ</math> (type <code>N_Vector**</code>). The operation returns 0 for success and a non-zero value otherwise.</p> |
| continued on next page      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |

| continued from last page        |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|---------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name                            | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| N_VLinearCombinationVectorArray | <p><code>ier = N_VLinearCombinationVectorArray(nv, ns, c, XX, Z);</code><br/> This routine computes the linear combination of <i>ns</i> vector arrays containing <i>nv</i> vectors with <i>n</i> elements:</p> $z_{j,i} = \sum_{k=1}^{ns} c_k x_{k,j,i}, \quad i = 1, \dots, n \quad j = 1, \dots, nv,$ <p>where <i>c</i> is an array of <i>ns</i> scalars (type <code>realtype*</code>), <i>XX</i> (type <code>N_Vector**</code>) is an array of <i>ns</i> vector arrays each containing <i>nv</i> vectors to be summed into the output vector array of <i>nv</i> vectors <i>ZZ</i> (type <code>N_Vector*</code>). If the output vector array <i>ZZ</i> is one of the vector arrays in <i>XX</i>, then it <i>must</i> be the first vector array in <i>XX</i>. The operation returns 0 for success and a non-zero value otherwise.</p> |

## 6.1 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.

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] )
```

The `NVECTOR_SERIAL` module defines serial implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4. Their names are obtained from those in Tables 6.2, 6.3, and 6.4. by appending the suffix `_Serial` (e.g. `N_VDestroy_Serial`). The module `NVECTOR_SERIAL` provides the following additional user-callable routines:

- N\_VNew\_Serial

This function creates and allocates memory for a serial `N_Vector`. Its only argument is the vector length.

```
N_Vector N_VNew_Serial(sunindextype vec_length);
```

- N\_VNewEmpty\_Serial

This function creates a new serial `N_Vector` with an empty (`NULL`) data array.

```
N_Vector N_VNewEmpty_Serial(sunindextype vec_length);
```

- N\_VMake\_Serial

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.)

```
N_Vector N_VMake_Serial(sunindextype vec_length, realtype *v_data);
```

- N\_VCloneVectorArray\_Serial

This function creates (by cloning) an array of count serial vectors.

```
N_Vector *N_VCloneVectorArray_Serial(int count, N_Vector w);
```

- N\_VCloneVectorArrayEmpty\_Serial

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

```
N_Vector *N_VCloneVectorArrayEmpty_Serial(int count, N_Vector w);
```

- N\_VDestroyVectorArray\_Serial

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`.

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

- N\_VGetLength\_Serial

This function returns the number of vector elements.

```
sunindextype N_VGetLength_Serial(N_Vector v);
```

- `N_VPrint_Serial`

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

```
void N_VPrint_Serial(N_Vector v);
```

- `N_VPrintFile_Serial`

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

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

## 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.

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

## 6.2 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;
    boolean_t 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.

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`.



- `N_VMake_Parallel`

This function creates and allocates memory for a parallel vector with user-provided data array. (This function does *not* allocate memory for `v_data` itself.)

```
N_Vector N_VMake_Parallel(MPI_Comm comm,
                          sunindextype local_length,
                          sunindextype global_length,
                          realtype *v_data);
```

- `N_VCloneVectorArray_Parallel`

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

```
N_Vector *N_VCloneVectorArray_Parallel(int count, N_Vector w);
```

- `N_VCloneVectorArrayEmpty_Parallel`

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

```
N_Vector *N_VCloneVectorArrayEmpty_Parallel(int count, N_Vector w);
```

- `N_VDestroyVectorArray_Parallel`

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`.

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

- `N_VGetLength_Parallel`

This function returns the number of vector elements (global vector length).

```
sunindextype N_VGetLength_Parallel(N_Vector v);
```

- `N_VGetLocalLength_Parallel`

This function returns the local vector length.

```
sunindextype N_VGetLocalLength_Parallel(N_Vector v);
```

- `N_VPrint_Parallel`

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

```
void N_VPrint_Parallel(N_Vector v);
```

- `N_VPrintFile_Parallel`

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

```
void N_VPrintFile_Parallel(N_Vector v, FILE *outfile);
```

## 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.

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



## 6.3 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;
    boolean_t 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 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] )
```

The `NVECTOR_OPENMP` module defines OpenMP implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4. Their names are obtained from those in Tables 6.2, 6.3, and 6.4 by appending the suffix `_OpenMP` (e.g. `N_VDestroy_OpenMP`). The module `NVECTOR_OPENMP` provides the following additional user-callable routines:

- `N_VNew_OpenMP`

This function creates and allocates memory for a OpenMP `N_Vector`. Arguments are the vector length and number of threads.

```
N_Vector N_VNew_OpenMP(sunindextype vec_length, int num_threads);
```

- `N_VNewEmpty_OpenMP`

This function creates a new OpenMP `N_Vector` with an empty (NULL) data array.

```
N_Vector N_VNewEmpty_OpenMP(sunindextype vec_length, int num_threads);
```

- `N_VMake_OpenMP`

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.)

```
N_Vector N_VMake_OpenMP(sunindextype vec_length, realtype *v_data, int num_threads);
```

- `N_VCloneVectorArray_OpenMP`

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

```
N_Vector *N_VCloneVectorArray_OpenMP(int count, N_Vector w);
```

- `N_VCloneVectorArrayEmpty_OpenMP`

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

```
N_Vector *N_VCloneVectorArrayEmpty_OpenMP(int count, N_Vector w);
```

- `N_VDestroyVectorArray_OpenMP`

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`.

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



- `N_VGetLength_OpenMP`

This function returns number of vector elements.

```
sunindextype N_VGetLength_OpenMP(N_Vector v);
```

- `N_VPrint_OpenMP`

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

```
void N_VPrint_OpenMP(N_Vector v);
```

- `N_VPrintFile_OpenMP`

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

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

### 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.



For solvers that include a Fortran interface module, the `NVECTOR_OPENMP` module also includes a Fortran-callable function `FN_VINITOMP(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.

## 6.4 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.

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] )
```

The NVECTOR\_PTHREADS module defines Pthreads implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4. Their names are obtained from those in Tables 6.2, 6.3, and 6.4 by appending the suffix `_Pthreads` (e.g. `N_VDestroy_Pthreads`). The module NVECTOR\_PTHREADS provides the following additional user-callable routines:

- **N\_VNew\_Pthreads**

This function creates and allocates memory for a Pthreads `N_Vector`. Arguments are the vector length and number of threads.

```
N_Vector N_VNew_Pthreads(sunindextype vec_length, int num_threads);
```

- **N\_VNewEmpty\_Pthreads**

This function creates a new Pthreads `N_Vector` with an empty (NULL) data array.

```
N_Vector N_VNewEmpty_Pthreads(sunindextype vec_length, int num_threads);
```

- **N\_VMake\_Pthreads**

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.)

```
N_Vector N_VMake_Pthreads(sunindextype vec_length, realtype *v_data, int num_threads);
```

- **N\_VCloneVectorArray\_Pthreads**

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

```
N_Vector *N_VCloneVectorArray_Pthreads(int count, N_Vector w);
```

- **N\_VCloneVectorArrayEmpty\_Pthreads**

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

```
N_Vector *N_VCloneVectorArrayEmpty_Pthreads(int count, N_Vector w);
```

- **N\_VDestroyVectorArray\_Pthreads**

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`.

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

- **N\_VGetLength\_Pthreads**

This function returns the number of vector elements.

```
sunindextype N_VGetLength_Pthreads(N_Vector v);
```

- **N\_VPrint\_Pthreads**

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



```
void N_VPrint_Pthreads(N_Vector v);
```

- **N\_VPrintFile\_Pthreads**

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

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

## 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. 

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

## 6.5 The NVECTOR\_PARHYP implementation

The NVECTOR\_PARHYP implementation of the NVECTOR module provided with SUNDIALS is a wrapper around *hypr*e's ParVector class. Most of the vector kernels simply call *hypr*e 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 `hypr_ParVector`, an MPI communicator, and a boolean flag *own\_parvector* indicating ownership of the *hypr*e parallel vector object *x*.

```
struct _N_VectorContent_ParHyp {
    sunindextype local_length;
    sunindextype global_length;
    booleantype own_parvector;
    MPI_Comm comm;
    hypr_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.

The NVECTOR\_PARHYP module defines implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4, except for `N_VSetArrayPointer` and `N_VGetArrayPointer`, because accessing raw vector data is handled by low-level *hypr*e 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 *hypr*e vector first, and then use *hypr*e methods to access the data. Usage examples of NVECTOR\_PARHYP are provided in the `cvAdvDiff_non_ph.c` example program for CVODE [27] and the `ark_diurnal_kry_ph.c` example program for ARKODE [34].

The names of parhyp methods are obtained from those in Tables 6.2, 6.3, and 6.4 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR\_PARHYP provides the following additional user-callable routines:

- `N_VNewEmpty_ParHyp`

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

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

- `N_VMake_ParHyp`

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

```
N_Vector N_VMake_ParHyp(hypr_ParVector *x);
```

- `N_VGetVector_ParHyp`

This function returns a pointer to the underlying *hypr*e vector.

```
hypr_ParVector *N_VGetVector_ParHyp(N_Vector v);
```

- `N_VCloneVectorArray_ParHyp`

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

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

- `N_VCloneVectorArrayEmpty_ParHyp`

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

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

- `N_VDestroyVectorArray_ParHyp`

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`.

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

- `N_VPrint_ParHyp`

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



```
void N_VPrint_ParHyp(N_Vector v);
```

- `N_VPrintFile_ParHyp`

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

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

#### Notes

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

## 6.6 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;
    boolean_t 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.

The NVECTOR\_PETSC module defines implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4, 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 [26].

The names of vector operations are obtained from those in Tables 6.2, 6.3, and 6.4 by appending the suffix `_Petsc` (e.g. `N_VDestroy_Petsc`). The module NVECTOR\_PETSC provides the following additional user-callable routines:

- `N_VNewEmpty_Petsc`

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_Vector N_VNewEmpty_Petsc(MPI_Comm comm,
                           sunindextype local_length,
                           sunindextype global_length);
```

- `N_VMake_Petsc`

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_Vector N_VMake_Petsc(Vec *pvec);
```

- `N_VGetVector_Petsc`

This function returns a pointer to the underlying PETSc vector.

```
Vec *N_VGetVector_Petsc(N_Vector v);
```

- `N_VCloneVectorArray_Petsc`

This function creates (by cloning) an array of `count` NVECTOR\_PETSC vectors.

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

- `N_VCloneVectorArrayEmpty_Petsc`

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

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

- `N_VDestroyVectorArray_Petsc`

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`.

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

- `N_VPrint_Petsc`

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

```
void N_VPrint_Petsc(N_Vector v);
```

- `N_VPrintFile_Petsc`

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

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

## 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.



## 6.7 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 namespace `suncudavec` manages vector data layout:

```
template <class T, class I>
class Vector {
    I size_;
    I mem_size_;
    T* h_vec_;
    T* d_vec_;
    StreamPartitioning<T, I>* partStream_;
    ReducePartitioning<T, I>* partReduce_;
    bool ownPartitioning_;

    ...
};
```

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 classes `StreamPartitioning` and `ReducePartitioning`, which handle thread partitioning for streaming and reduction vector kernels, respectively, and a boolean flag that signals if the vector owns the thread partitioning. The class `Vector` inherits from the empty structure

```
struct _N_VectorContent_Cuda {
};
```

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 `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.

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

Unlike other native `SUNDIALS` vector types, `NVECTOR_CUDA` does not provide macros to access its member variables.



The NVECTOR\_CUDA module defines implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4, except for `N_VGetArrayPointer` and `N_VSetArrayPointer`. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor with SUNDIALS direct solvers and preconditioners. This support will be added in subsequent SUNDIALS releases. The NVECTOR\_CUDA module provides separate functions to access data on the host and on the device. It also provides methods for copying from the host to the device and vice versa. Usage examples of NVECTOR\_CUDA are provided in some example programs for CVOID [27].

The names of vector operations are obtained from those in Tables 6.2, 6.3, and 6.4 by appending the suffix `_Cuda` (e.g. `N_VDestroy_Cuda`). The module NVECTOR\_CUDA provides the following additional user-callable routines:

- `N_VNew_Cuda`

This function creates and allocates memory for a CUDA `N_Vector`. The memory is allocated on both host and device. Its only argument is the vector length.

```
N_Vector N_VNew_Cuda(sunindextype vec_length);
```

- `N_VNewEmpty_Cuda`

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_Vector N_VNewEmpty_Cuda(sunindextype vec_length);
```

- `N_VMake_Cuda`

This function creates and allocates memory for an NVECTOR\_CUDA wrapper around a user-provided `suncudavec::Vector` class. Its only argument is of type `N_VectorContent_Cuda`, which is the pointer to the class.

```
N_Vector N_VMake_Cuda(N_VectorContent_Cuda c);
```

- `N_VCloneVectorArray_Cuda`

This function creates (by cloning) an array of `count` NVECTOR\_CUDA vectors.

```
N_Vector *N_VCloneVectorArray_Cuda(int count, N_Vector w);
```

- `N_VCloneVectorArrayEmpty_Cuda`

This function creates (by cloning) an array of `count` NVECTOR\_CUDA vectors, each with pointers to CUDA vectors set to (NULL).

```
N_Vector *N_VCloneVectorArrayEmpty_Cuda(int count, N_Vector w);
```

- `N_VDestroyVectorArray_Cuda`

This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Cuda` or with `N_VCloneVectorArrayEmpty_Cuda`.

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

- `N_VGetLength_Cuda`

This function returns the length of the vector.

```
sunindextype N_VGetLength_Cuda(N_Vector v);
```



- `N_VGetHostArrayPointer_Cuda`  
This function returns a pointer to the vector data on the host.  
`realtype *N_VGetHostArrayPointer_Cuda(N_Vector v);`
- `N_VGetDeviceArrayPointer_Cuda`  
This function returns a pointer to the vector data on the device.  
`realtype *N_VGetDeviceArrayPointer_Cuda(N_Vector v);`
- `N_VCopyToDevice_Cuda`  
This function copies host vector data to the device.  
`realtype *N_VCopyToDevice_Cuda(N_Vector v);`
- `N_VCopyFromDevice_Cuda`  
This function copies vector data from the device to the host.  
`realtype *N_VCopyFromDevice_Cuda(N_Vector v);`
- `N_VPrint_Cuda`  
This function prints the content of a CUDA vector to `stdout`.  
`void N_VPrint_Cuda(N_Vector v);`
- `N_VPrintFile_Cuda`  
This function prints the content of a CUDA vector to `outfile`.  
`void N_VPrintFile_Cuda(N_Vector v, FILE *outfile);`

#### 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`.
- 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.



## 6.8 The NVECTOR\_RAJA implementation

The NVECTOR\_RAJA module is an experimental NVECTOR implementation using the RAJA hardware abstraction layer, <https://software.llnl.gov/RAJA/>. 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 OpenAC. 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, and pointers to vector data on the host and 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 `sunraja::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `sunraja::Vector` class without requiring changes to the user API.

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

Unlike other native SUNDIALS vector types, NVECTOR\_RAJA does not provide macros to access its member variables.

The NVECTOR\_RAJA module defines the implementations of all vector operations listed in Tables 6.2, 6.3, and 6.4, 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 vector `N_VGetArrayPointer` and `N_VSetArrayPointer` are not implemented by the RAJA vector. As such, this vector cannot be used with SUNDIALS Fortran interfaces, nor with 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 [27].

The names of vector operations are obtained from those in Tables 6.2, 6.3, and 6.4, by appending the suffix `_Raja` (e.g. `N_VDestroy_Raja`). The module NVECTOR\_RAJA provides the following additional user-callable routines:

- `N_VNew_Raja`

This function creates and allocates memory for a RAJA `N_Vector`. The memory is allocated on both the host and the device. Its only argument is the vector length.

```
N_Vector N_VNew_Raja(sunindextype vec_length);
```

- `N_VNewEmpty_Raja`

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_Vector N_VNewEmpty_Raja(sunindextype vec_length);
```

- `N_VMake_Raja`

This function creates and allocates memory for an NVECTOR\_RAJA wrapper around a user-provided `sunraja::Vector` class. Its only argument is of type `N_VectorContent_Raja`, which is the pointer to the class.

```
N_Vector N_VMake_Raja(N_VectorContent_Raja c);
```

- `N_VCloneVectorArray_Raja`

This function creates (by cloning) an array of `count` NVECTOR\_RAJA vectors.

```
N_Vector *N_VCloneVectorArray_Raja(int count, N_Vector w);
```

- `N_VCloneVectorArrayEmpty_Raja`

This function creates (by cloning) an array of `count` NVECTOR\_RAJA vectors, each with pointers to RAJA vectors set to (NULL).

```
N_Vector *N_VCloneVectorArrayEmpty_Raja(int count, N_Vector w);
```

- `N_VDestroyVectorArray_Raja`

This function frees memory allocated for the array of `count` variables of type `N_Vector` created with `N_VCloneVectorArray_Raja` or with `N_VCloneVectorArrayEmpty_Raja`.

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

- `N_VGetLength_Raja`

This function returns the length of the vector.

```
sunindextype N_VGetLength_Raja(N_Vector v);
```

- `N_VGetHostArrayPointer_Raja`

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

```
realtype *N_VGetHostArrayPointer_Raja(N_Vector v);
```

- `N_VGetDeviceArrayPointer_Raja`

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

```
realtype *N_VGetDeviceArrayPointer_Raja(N_Vector v);
```

- `N_VCopyToDevice_Raja`

This function copies host vector data to the device.

```
realtype *N_VCopyToDevice_Raja(N_Vector v);
```

- `N_VCopyFromDevice_Raja`

This function copies vector data from the device to the host.

```
realtype *N_VCopyFromDevice_Raja(N_Vector v);
```

- `N_VPrint_Raja`

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

```
void N_VPrint_Raja(N_Vector v);
```

- `N_VPrintFile_Raja`

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

```
void N_VPrintFile_Raja(N_Vector v, FILE *outfile);
```

## 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.



## 6.9 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_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:  $Z[i] = c[0] X[0][i] + c[1] X[1][i] + c[2] X[2][i]$

## 6.10 NVECTOR functions used by CVODE

In Table 6.5 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 CVDLS stands for the direct linear solver interface in CVODE; CVSPILS stands for the scaled, preconditioned, iterative 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.

Table 6.5: List of vector functions usage by CVODE code modules

|                      | CVODE | CVDLS | CVDIAG | CVSPILS | CVBANDPRE | CVBBDPRE | FCVODE |
|----------------------|-------|-------|--------|---------|-----------|----------|--------|
| N_VGetVectorID       |       |       |        |         |           |          |        |
| N_VClone             | ✓     |       | ✓      | ✓       |           |          |        |
| N_VCloneEmpty        |       |       |        |         |           |          | ✓      |
| N_VDestroy           | ✓     |       | ✓      | ✓       |           |          |        |
| N_VSpace             | ✓     |       |        |         |           |          |        |
| N_VGetArrayPointer   |       | ✓     |        |         | ✓         | ✓        | ✓      |
| N_VSetArrayPointer   |       | ✓     |        |         |           |          | ✓      |
| N_VLinearSum         | ✓     | ✓     | ✓      | ✓       |           |          |        |
| N_VConst             | ✓     |       |        | ✓       |           |          |        |
| N_VProd              | ✓     |       | ✓      | ✓       |           |          |        |
| N_VDiv               | ✓     |       | ✓      | ✓       |           |          |        |
| N_VScale             | ✓     | ✓     | ✓      | ✓       | ✓         | ✓        |        |
| N_VAbs               | ✓     |       |        |         |           |          |        |
| N_VInv               | ✓     |       | ✓      |         |           |          |        |
| N_VAddConst          | ✓     |       | ✓      |         |           |          |        |
| N_VDotProd           |       |       |        | ✓       |           |          |        |
| N_VMaxNorm           | ✓     |       |        |         |           |          |        |
| N_VWrmsNorm          | ✓     | ✓     |        | ✓       | ✓         | ✓        |        |
| N_VMin               | ✓     |       |        |         |           |          |        |
| N_VCompare           |       |       | ✓      |         |           |          |        |
| N_VInvTest           |       |       | ✓      |         |           |          |        |
| N_VLinearCombination | ✓     |       |        | ✓       |           |          |        |
| N_VScaleAddMulti     | ✓     |       |        |         |           |          |        |
| N_VDotProdMulti      |       |       | ✓      |         |           |          |        |
| N_VScaleVectorArray  | ✓     |       |        |         |           |          |        |

The vector functions listed in Table 6.2 that are *not* used by CVODE are: N\_VWL2Norm, N\_VL1Norm, N\_VWrmsNormMask, N\_VConstrMask, and N\_VMinQuotient. Therefore, a user-supplied NVECTOR module for CVODE could omit these functions.

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





## 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.

The generic `SUNMatrix` type has been modeled after the object-oriented style of the generic `N_Vector` type. Specifically, a generic `SUNMatrix` is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the matrix, and an *ops* field pointing to a structure with generic matrix operations. The type `SUNMatrix` is defined as

```
typedef struct _generic_SUNMatrix *SUNMatrix;
```

```
struct _generic_SUNMatrix {  
    void *content;  
    struct _generic_SUNMatrix_Ops *ops;  
};
```

The `_generic_SUNMatrix_Ops` structure is essentially a list of pointers to the various actual matrix operations, and is defined as

```
struct _generic_SUNMatrix_Ops {  
    SUNMatrix_ID (*getid)(SUNMatrix);  
    SUNMatrix (*clone)(SUNMatrix);  
    void (*destroy)(SUNMatrix);  
    int (*zero)(SUNMatrix);  
    int (*copy)(SUNMatrix, SUNMatrix);  
    int (*scaleadd)(realtype, SUNMatrix, SUNMatrix);  
    int (*scaleaddi)(realtype, SUNMatrix);  
    int (*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

Table 7.1: 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_CUSTOM | User-provided custom matrix             | 3        |

illustrate this point we show below the implementation of a typical matrix operation from the generic SUNMATRIX module, namely `SUNMatZero`, which sets all values of a matrix `A` to zero, returning a flag denoting a successful/failed operation:

```
int SUNMatZero(SUNMatrix A)
{
    return((int) A->ops->zero(A));
}
```

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

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

Table 7.2: Description of the `SUNMatrix` operations

| Name                          | Usage and Description                                                                                                                                                                                                                                                                                                                                                                   |
|-------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUNMatGetID                   | <pre>id = SUNMatGetID(A);</pre> <p>Returns the type identifier for the matrix <code>A</code>. It is used to determine the matrix implementation type (e.g. dense, banded, sparse, . . .) from the abstract <code>SUNMatrix</code> interface. This is used to assess compatibility with SUNDIALS-provided linear solver implementations. Returned values are given in the Table 7.1.</p> |
| <i>continued on next page</i> |                                                                                                                                                                                                                                                                                                                                                                                         |

| Name            | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUNMatClone     | <pre>B = SUNMatClone(A);</pre> <p>Creates a new <b>SUNMatrix</b> of the same type as an existing matrix <b>A</b> and sets the <i>ops</i> field. It does not copy the matrix, but rather allocates storage for the new matrix.</p>                                                                                                                                                                                                                                                                                                                                         |
| SUNMatDestroy   | <pre>SUNMatDestroy(A);</pre> <p>Destroys the <b>SUNMatrix</b> <b>A</b> and frees memory allocated for its internal data.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| SUNMatSpace     | <pre>ier = SUNMatSpace(A, &amp;lrw, &amp;liw);</pre> <p>Returns the storage requirements for the matrix <b>A</b>. <b>lrw</b> is a <b>long int</b> containing the number of realtype words and <b>liw</b> is a <b>long int</b> containing the number of integer words. The return value is an integer flag denoting success/failure of the operation.</p> <p>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 <b>SUNMATRIX</b> module if that information is not of interest.</p> |
| SUNMatZero      | <pre>ier = SUNMatZero(A);</pre> <p>Performs the operation <math>A_{ij} = 0</math> for all entries of the matrix <i>A</i>. The return value is an integer flag denoting success/failure of the operation.</p>                                                                                                                                                                                                                                                                                                                                                              |
| SUNMatCopy      | <pre>ier = SUNMatCopy(A,B);</pre> <p>Performs the operation <math>B_{ij} = A_{i,j}</math> for all entries of the matrices <i>A</i> and <i>B</i>. The return value is an integer flag denoting success/failure of the operation.</p>                                                                                                                                                                                                                                                                                                                                       |
| SUNMatScaleAdd  | <pre>ier = SUNMatScaleAdd(c, A, B);</pre> <p>Performs the operation <math>A = cA + B</math>. The return value is an integer flag denoting success/failure of the operation.</p>                                                                                                                                                                                                                                                                                                                                                                                           |
| SUNMatScaleAddI | <pre>ier = SUNMatScaleAddI(c, A);</pre> <p>Performs the operation <math>A = cA + I</math>. The return value is an integer flag denoting success/failure of the operation.</p>                                                                                                                                                                                                                                                                                                                                                                                             |
| SUNMatMatvec    | <pre>ier = SUNMatMatvec(A, x, y);</pre> <p>Performs the matrix-vector product operation, <math>y = Ax</math>. It should only be called with vectors <b>x</b> and <b>y</b> that are compatible with the matrix <b>A</b> – both in storage type and dimensions. The return value is an integer flag denoting success/failure of the operation.</p>                                                                                                                                                                                                                          |

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            | ✓      |                | ✓      | ✓        |           |            |      |      | ✓           |

*continued on next page*

| Matrix Interface | Serial | Parallel (MPI) | OpenMP | pThreads | hybre Vec. | PETSc Vec. | CUDA | RAJA | User Suppl. |
|------------------|--------|----------------|--------|----------|------------|------------|------|------|-------------|
| Band             | ✓      |                | ✓      | ✓        |            |            |      |      | ✓           |
| Sparse           | ✓      |                | ✓      | ✓        |            |            |      |      | ✓           |
| User supplied    | ✓      | ✓              | ✓      | ✓        | ✓          | ✓          | ✓    | ✓    | ✓           |

## 7.1 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.

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\_LDATAL\_D**

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

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

Implementation:

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

- `SM_DATA_D` and `SM_COLS_D`

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

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

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

Implementation:

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

- `SM_COLUMN_D` and `SM_ELEMENT_D`

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

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

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

Implementation:

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

The `SUNMATRIX_DENSE` module defines dense implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Dense` (e.g. `SUNMatCopy_Dense`). The module `SUNMATRIX_DENSE` provides the following additional user-callable routines:

- `SUNDenseMatrix`

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.

```
SUNMatrix SUNDenseMatrix(sunindextype M, sunindextype N);
```

- `SUNDenseMatrix.Print`

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.

```
void SUNDenseMatrix_Print(SUNMatrix A, FILE* outfile);
```

- **SUNDenseMatrix.Rows**  
This function returns the number of rows in the dense **SUNMatrix**.  
`sunindextype SUNDenseMatrix_Rows(SUNMatrix A);`
- **SUNDenseMatrix.Columns**  
This function returns the number of columns in the dense **SUNMatrix**.  
`sunindextype SUNDenseMatrix_Columns(SUNMatrix A);`
- **SUNDenseMatrix.LData**  
This function returns the length of the data array for the dense **SUNMatrix**.  
`sunindextype SUNDenseMatrix_LData(SUNMatrix A);`
- **SUNDenseMatrix.Data**  
This function returns a pointer to the data array for the dense **SUNMatrix**.  
`realtype* SUNDenseMatrix_Data(SUNMatrix A);`
- **SUNDenseMatrix.Cols**  
This function returns a pointer to the cols array for the dense **SUNMatrix**.  
`realtype** SUNDenseMatrix_Cols(SUNMatrix A);`
- **SUNDenseMatrix.Column**  
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.  
`realtype* SUNDenseMatrix_Column(SUNMatrix A, sunindextype j);`

## 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.

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.

## 7.2 The SUNMatrix\_Band implementation

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

```
struct _SUNMatrixContent_Band {
    sunindextype M;
    sunindextype N;
    sunindextype mu;
    sunindextype ml;
    sunindextype s_mu;
    sunindextype ldim;
    realtype *data;
    sunindextype ldata;
    realtype **cols;
};
```

A diagram of the underlying data representation in a banded matrix is shown in Figure 7.1. A more complete description of the parts of this *content* field is given below:

**M** - number of rows

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

**mu** - upper half-bandwidth,  $0 \leq \mu < N$

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

**s\_mu** - storage upper bandwidth,  $\mu \leq s\_mu < N$ . The LU decomposition routines in the associated SUNLINSOL\_BAND and SUNLINSOL\_LAPACKBAND modules write the LU factors into the storage for A. The upper triangular factor U, however, may have an upper bandwidth as big as  $\min(N-1, \mu+ml)$  because of partial pivoting. The **s\_mu** field holds the upper half-bandwidth allocated for A.

**ldim** - leading dimension ( $ldim \geq s\_mu+ml+1$ )

**data** - pointer to a contiguous block of **realtype** variables. The elements of the banded matrix are stored columnwise (i.e. columns are stored one on top of the other in memory). Only elements within the specified half-bandwidths are stored. **data** is a pointer to **ldata** contiguous locations which hold the elements within the band of A.

**ldata** - length of the data array ( $= ldim \cdot N$ )

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

The header file to include when using this module is **sunmatrix/sunmatrix.band.h**. The SUNMATRIX\_BAND module is accessible from all SUNDIALS solvers *without* linking to the **libsundials\_sunmatrixband** module library.

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.

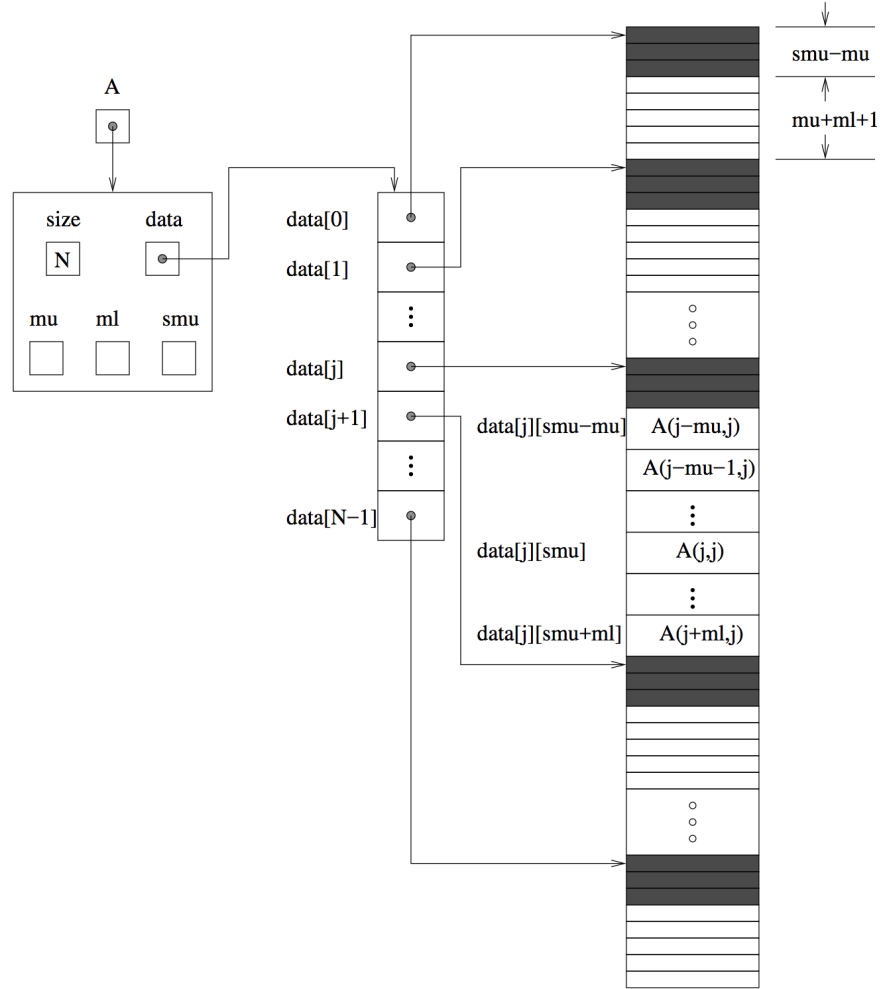


Figure 7.1: Diagram of the storage for the `SUNMATRIX_BAND` module. Here  $A$  is an  $N \times N$  band matrix with upper and lower half-bandwidths  $\mu$  and  $ml$ , respectively. The rows and columns of  $A$  are numbered from 0 to  $N - 1$  and the  $(i, j)$ -th element of  $A$  is denoted  $A(i, j)$ . The greyed out areas of the underlying component storage are used by the associated `SUNLINSOL_BAND` linear solver.



- **SM\_CONTENT\_B**

This routine gives access to the contents of the banded **SUNMatrix**.

The assignment **A\_cont** = **SM\_CONTENT\_B(A)** sets **A\_cont** to be a pointer to the banded **SUNMatrix** content structure.

Implementation:

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

- **SM\_ROWS\_B**, **SM\_COLUMNS\_B**, **SM\_UBAND\_B**, **SM\_LBAND\_B**, **SM\_SUBAND\_B**, **SM\_LDIM\_B**, and **SM\_LDATA\_B**

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

These may be used either to retrieve or to set these values. For example, the assignment **A\_rows** = **SM\_ROWS\_B(A)** sets **A\_rows** to be the number of rows in the matrix **A**. Similarly, the assignment **SM\_COLUMNS\_B(A)** = **A\_cols** sets the number of columns in **A** to equal **A\_cols**.

Implementation:

```
#define SM_ROWS_B(A)         ( SM_CONTENT_B(A)->M )
#define SM_COLUMNS_B(A)      ( SM_CONTENT_B(A)->N )
#define SM_UBAND_B(A)        ( SM_CONTENT_B(A)->mu )
#define SM_LBAND_B(A)        ( SM_CONTENT_B(A)->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_SUBBAND_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_SUBBAND_B(A)] )
```

The `SUNMATRIX_BAND` module defines banded implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Band` (e.g. `SUNMatCopy_Band`). The module `SUNMATRIX_BAND` provides the following additional user-callable routines:

- **SUNBandMatrix**

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.

```
SUNMatrix SUNBandMatrix(sunindextype N, sunindextype mu,
                        sunindextype ml, sunindextype smu);
```

- **SUNBandMatrix.Print**

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.

```
void SUNBandMatrix_Print(SUNMatrix A, FILE* outfile);
```

- **SUNBandMatrix.Rows**

This function returns the number of rows in the banded **SUNMatrix**.

```
sunindextype SUNBandMatrix_Rows(SUNMatrix A);
```

- **SUNBandMatrix.Columns**

This function returns the number of columns in the banded **SUNMatrix**.

```
sunindextype SUNBandMatrix_Columns(SUNMatrix A);
```

- **SUNBandMatrix.LowerBandwidth**

This function returns the lower half-bandwidth of the banded **SUNMatrix**.

```
sunindextype SUNBandMatrix_LowerBandwidth(SUNMatrix A);
```

- **SUNBandMatrix.UpperBandwidth**

This function returns the upper half-bandwidth of the banded **SUNMatrix**.

```
sunindextype SUNBandMatrix_UpperBandwidth(SUNMatrix A);
```

- **SUNBandMatrix.StoredUpperBandwidth**

This function returns the stored upper half-bandwidth of the banded **SUNMatrix**.

```
sunindextype SUNBandMatrix_StoredUpperBandwidth(SUNMatrix A);
```

- `SUNBandMatrix_LDim`

This function returns the length of the leading dimension of the banded `SUNMatrix`.

```
sunindextype SUNBandMatrix_LDim(SUNMatrix A);
```

- `SUNBandMatrix_Data`

This function returns a pointer to the data array for the banded `SUNMatrix`.

```
realtype* SUNBandMatrix_Data(SUNMatrix A);
```

- `SUNBandMatrix_Cols`

This function returns a pointer to the cols array for the banded `SUNMatrix`.

```
realtype** SUNBandMatrix_Cols(SUNMatrix A);
```

- `SUNBandMatrix_Column`

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  $m$ .

```
realtype* SUNBandMatrix_Column(SUNMatrix A, sunindextype j);
```

#### 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.



For solvers that include a Fortran interface module, the `SUNMATRIX_BAND` module also includes the Fortran-callable function `FSUNBandMatInit(code, N, mu, ml, smu, 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`, `ml` and `smu` are the corresponding band matrix construction arguments (declared to match C type `long int`); and `ier` is an error return flag equal to 0 for success and -1 for failure. Both `code` and `ier` are declared to match C type `int`. Additionally, when using `ARKODE` with a non-identity mass matrix, the Fortran-callable function `FSUNBandMassMatInit(N, mu, ml, smu, ier)` initializes this `SUNMATRIX_BAND` module for storing the mass matrix.

## 7.3 The SUNMatrix\_Sparse implementation

The sparse implementation of the `SUNMATRIX` module provided with `SUNDIALS`, `SUNMATRIX_SPARSE`, is designed to work with either *compressed-sparse-column* (CSC) or *compressed-sparse-row* (CSR) sparse matrix formats. To this end, it defines the *content* field of `SUNMatrix` to be the following structure:

```

struct _SUNMatrixContent_Sparse {
    sunindextype M;
    sunindextype N;
    sunindextype NNZ;
    sunindextype NP;
    realtype *data;
    int sparsetype;
    sunindextype *indexvals;
    sunindextype *indexptrs;
    /* CSC indices */
    sunindextype **rowvals;
    sunindextype **colptrs;
    /* CSR indices */
    sunindextype **colvals;
    sunindextype **rowptrs;
};

```

A diagram of the underlying data representation for a CSC matrix is shown in Figure 7.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

**M** - number of rows

**N** - number of columns

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

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

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

**sparsetype** - type of the sparse matrix (**CSC\_MAT** or **CSR\_MAT**)

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

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

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

**rowvals** - pointer to **indexvals** when **sparsetype** is **CSC\_MAT**, otherwise set to **NULL**.

**colptrs** - pointer to **indexptrs** when **sparsetype** is **CSC\_MAT**, otherwise set to **NULL**.

**colvals** - pointer to **indexvals** when **sparsetype** is **CSR\_MAT**, otherwise set to **NULL**.

**rowptrs** - pointer to **indexptrs** when **sparsetype** is **CSR\_MAT**, otherwise set to **NULL**.

For example, the  $5 \times 4$  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.

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

- `SM_CONTENT_S`

This routine gives access to the contents of the sparse `SUNMatrix`.

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

Implementation:

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

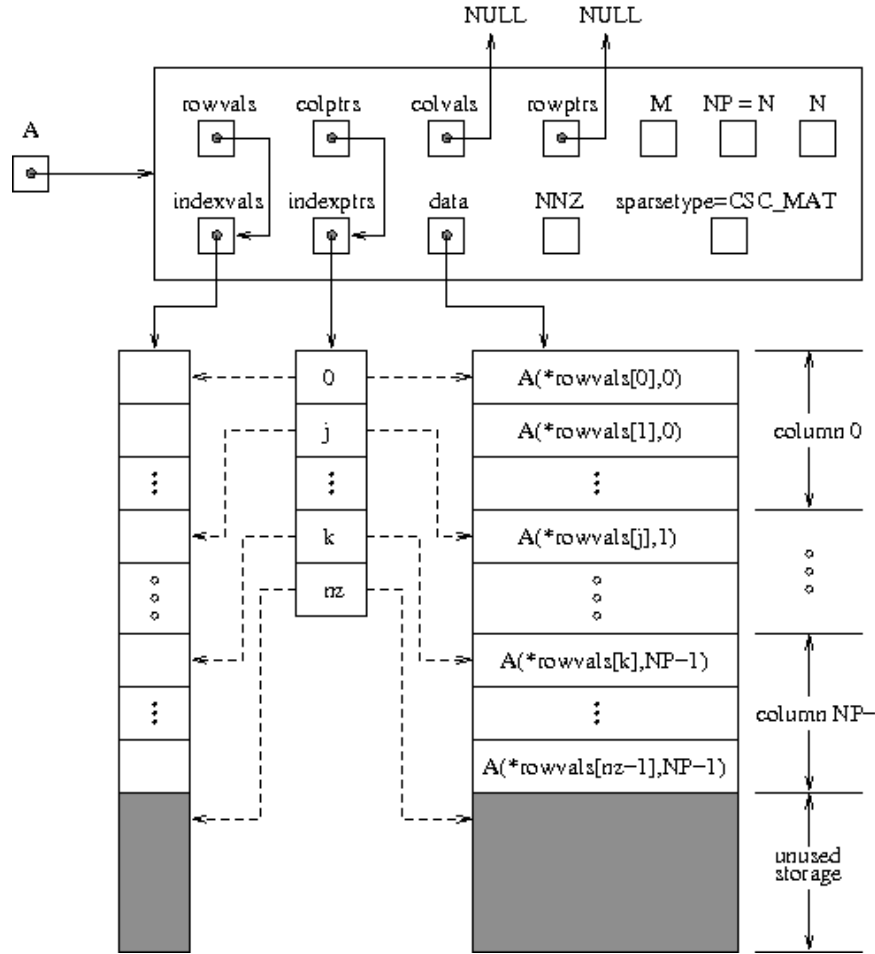


Figure 7.2: Diagram of the storage for a compressed-sparse-column matrix. Here  $A$  is an  $M \times N$  sparse matrix with storage for up to  $NNZ$  nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to  $M - 1$ , corresponding 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.

- `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 )
```

The `SUNMATRIX_SPARSE` module defines sparse implementations of all matrix operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Sparse` (e.g. `SUNMatCopy_Sparse`). The module `SUNMATRIX_SPARSE` provides the following additional user-callable routines:

- `SUNSparseMatrix`

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`).

```
SUNMatrix SUNSparseMatrix(sunindextype M, sunindextype N,
                          sunindextype NNZ, int sparsetype);
```

- `SUNSparseFromDenseMatrix`

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.

```
SUNMatrix SUNSparseFromDenseMatrix(SUNMatrix A, realtype droptol,
                                   int sparsetype);
```

- **SUNSparseFromBandMatrix**

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.

```
SUNMatrix SUNSparseFromBandMatrix(SUNMatrix A, realtype droptol,
                                   int sparsetype);
```

- **SUNSparseMatrix\_Realloc**

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).

```
int SUNSparseMatrix_Realloc(SUNMatrix A);
```

- **SUNSparseMatrix\_Reallocate**

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).

```
int SUNSparseMatrix_Reallocate(SUNMatrix A, sunindextype NNZ);
```

- **SUNSparseMatrix\_Print**

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.

```
void SUNSparseMatrix_Print(SUNMatrix A, FILE* outfile);
```

- **SUNSparseMatrix\_Rows**

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

```
sunindextype SUNSparseMatrix_Rows(SUNMatrix A);
```

- **SUNSparseMatrix\_Columns**

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

```
sunindextype SUNSparseMatrix_Columns(SUNMatrix A);
```



- `SUNSparseMatrix_NNZ`

This function returns the number of entries allocated for nonzero storage for the sparse matrix `SUNMatrix`.

```
sunindextype SUNSparseMatrix_NNZ(SUNMatrix A);
```

- `SUNSparseMatrix_NP`

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.

```
sunindextype SUNSparseMatrix_NP(SUNMatrix A);
```

- `SUNSparseMatrix_SparseType`

This function returns the storage type (`CSR_MAT` or `CSC_MAT`) for the sparse `SUNMatrix`.

```
int SUNSparseMatrix_SparseType(SUNMatrix A);
```

- `SUNSparseMatrix_Data`

This function returns a pointer to the data array for the sparse `SUNMatrix`.

```
realtype* SUNSparseMatrix_Data(SUNMatrix A);
```

- `SUNSparseMatrix_IndexValues`

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.

```
sunindextype* SUNSparseMatrix_IndexValues(SUNMatrix A);
```

- `SUNSparseMatrix_IndexPointers`

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.

```
sunindextype* SUNSparseMatrix_IndexPointers(SUNMatrix A);
```

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

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.



## 7.4 SUNMatrix Examples

There are `SUNMatrix` examples that may be installed for each implementation: dense, banded, and sparse. Each implementation makes use of the functions in `test_sunmatrix.c`. These example functions show simple usage of the `SUNMatrix` family of functions. The inputs to the examples depend on the matrix 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_sunmatrix.c`:

- **Test\_SUNMatGetID**: Verifies the returned matrix ID against the value that should be returned.
- **Test\_SUNMatClone**: Creates clone of an existing matrix, copies the data, and checks that their values match.
- **Test\_SUNMatZero**: Zeros out an existing matrix and checks that each entry equals 0.0.
- **Test\_SUNMatCopy**: Clones an input matrix, copies its data to a clone, and verifies that all values match.
- **Test\_SUNMatScaleAdd**: Given an input matrix  $A$  and an input identity matrix  $I$ , this test clones and copies  $A$  to a new matrix  $B$ , computes  $B = -B + B$ , and verifies that the resulting matrix entries equal 0.0. Additionally, if the matrix is square, this test clones and copies  $A$  to a new matrix  $D$ , clones and copies  $I$  to a new matrix  $C$ , computes  $D = D + I$  and  $C = C + A$  using **SUNMatScaleAdd**, and then verifies that  $C == D$ .
- **Test\_SUNMatScaleAddI**: Given an input matrix  $A$  and an input identity matrix  $I$ , this clones and copies  $I$  to a new matrix  $B$ , computes  $B = -B + I$  using **SUNMatScaleAddI**, and verifies that the resulting matrix entries equal 0.0.
- **Test\_SUNMatMatvec**: Given an input matrix  $A$  and input vectors  $x$  and  $y$  such that  $y = Ax$ , this test has different behavior depending on whether  $A$  is square. If it is square, it clones and copies  $A$  to a new matrix  $B$ , computes  $B = 3B + I$  using **SUNMatScaleAddI**, clones  $y$  to new vectors  $w$  and  $z$ , computes  $z = Bx$  using **SUNMatMatvec**, computes  $w = 3y + x$  using **N\_VLinearSum**, and verifies that  $w == z$ . If  $A$  is not square, it just clones  $y$  to a new vector  $z$ , computes  $z = Ax$  using **SUNMatMatvec**, and verifies that  $y == z$ .
- **Test\_SUNMatSpace** verifies that **SUNMatSpace** can be called, and outputs the results to **stdout**.

## 7.5 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. Neither the main CVODE integrator or the CVSPILS interface call SUNMATRIX functions directly, so the table columns are specific to the CVDLS direct solver interface and the CVBANDPRE and CVBBDPRE preconditioner modules.

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

|                        | CVDLS | CVBANDPRE | CVBBDPRE |
|------------------------|-------|-----------|----------|
| <b>SUNMatGetID</b>     | ✓     |           |          |
| <b>SUNMatClone</b>     | ✓     |           |          |
| <b>SUNMatDestroy</b>   | ✓     | ✓         | ✓        |
| <b>SUNMatZero</b>      | ✓     | ✓         | ✓        |
| <b>SUNMatCopy</b>      | ✓     | ✓         | ✓        |
| <b>SUNMatScaleAddI</b> | ✓     | ✓         | ✓        |
| <b>SUNMatSpace</b>     | †     | †         | †        |

The matrix functions listed in Table 7.2 with a † symbol are optionally used, in that these are only called if they are implemented in the SUNMATRIX module that is being used (i.e. their function pointers are non-NULL). The matrix functions listed in Table 7.2 that are *not* used by CVODE are: `SUNMatScaleAdd` and `SUNMatMatvec`. Therefore a user-supplied SUNMATRIX module for CVODE could omit these functions.



## Chapter 8

# Description of the SUNLinearSolver module

For problems that involve the solution of linear systems of equations, the SUNDIALS solvers operate using generic linear solver modules (of type `SUNLinearSolver`), through a set of operations defined by the particular SUNLINSOL implementation. These 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 methods. Moreover, users can provide their own specific SUNLINSOL implementation to each SUNDIALS solver, particularly in cases where they provide their own NVECTOR and/or SUNMATRIX modules, and the customized linear solver leverages these additional data structures to create highly efficient and/or scalable solvers for their particular problem. Additionally, SUNDIALS provides native implementations SUNLINSOL modules, as well as SUNLINSOL modules that interface between SUNDIALS and external linear solver libraries.

The various SUNDIALS solvers have been designed to specifically leverage the use of either *direct linear solvers* or *scaled, preconditioned, iterative linear solvers*, through their “Dls” and “Spils” interfaces, respectively. Additionally, SUNDIALS solvers can make use of user-supplied custom linear solvers, whether these are problem-specific or come from external solver libraries.

For iterative (and possibly custom) linear solvers, the SUNDIALS solvers 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, we 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 SUNDIALS solvers request that iterative linear solvers stop based on the 2-norm of the scaled preconditioned residual meeting a prescribed tolerance

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

We note that not all of the iterative linear solvers implemented in SUNDIALS support the full range of the above options. Similarly, some of the SUNDIALS integrators only utilize a subset of these options. Exceptions to the operators shown above are described in the documentation for each SUNLINSOL implementation, or for each SUNDIALS solver “Spils” interface.

The generic `SUNLinearSolver` type has been modeled after the object-oriented style of the generic `N_Vector` type. Specifically, a generic `SUNLinearSolver` is a pointer to a structure that has an implementation-dependent *content* field containing the description and actual data of the linear solver, and an *ops* field pointing to a structure with generic linear solver operations. The type `SUNLinearSolver` is defined as

```
typedef struct _generic_SUNLinearSolver *SUNLinearSolver;
```

```
struct _generic_SUNLinearSolver {
    void *content;
    struct _generic_SUNLinearSolver_Ops *ops;
};
```

The `_generic_SUNLinearSolver_Ops` structure is essentially a list of pointers to the various actual linear solver operations, and is defined as

```
struct _generic_SUNLinearSolver_Ops {
    SUNLinearSolver_Type (*gettype)(SUNLinearSolver);
    int (*setatimes)(SUNLinearSolver, void*, ATimesFn);
    int (*setpreconditioner)(SUNLinearSolver, void*,
                             PSetupFn, PSolveFn);
    int (*setscalingvectors)(SUNLinearSolver,
                             N_Vector, N_Vector);
    int (*initialize)(SUNLinearSolver);
    int (*setup)(SUNLinearSolver, SUNMatrix);
    int (*solve)(SUNLinearSolver, SUNMatrix, N_Vector,
                 N_Vector, realtype);
    int (*numiters)(SUNLinearSolver);
    realtype (*resnorm)(SUNLinearSolver);
    long int (*lastflag)(SUNLinearSolver);
    int (*space)(SUNLinearSolver, long int*, long int*);
    N_Vector (*resid)(SUNLinearSolver);
    int (*free)(SUNLinearSolver);
};
```

The generic SUNLINSOL module defines and implements the linear solver operations acting on `SUNLinearSolver` objects. These routines are in fact only wrappers for 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));
}
```

Table 8.2 contains a complete list of all linear solver operations defined by the generic SUNLINSOL module. In order to support both direct and iterative linear solver types, the generic SUNLINSOL module defines linear solver routines (or arguments) that may be specific to individual use cases. As such, for each routine we specify its intended use. If a custom SUNLINSOL module is provided, the function pointers for non-required routines may be set to NULL to indicate that they are not provided.

A particular implementation of the SUNLINSOL module must:

Table 8.1: Identifiers associated with linear solver kernels supplied with SUNDIALS.

| Linear Solver ID          | Solver type       | ID Value |
|---------------------------|-------------------|----------|
| SUNLINEARSOLVER_DIRECT    | Direct solvers    | 0        |
| SUNLINEARSOLVER_ITERATIVE | Iterative solvers | 1        |
| SUNLINEARSOLVER_CUSTOM    | Custom solvers    | 2        |

- Specify the *content* field of the `SUNLinearSolver` object.
- Define and implement a minimal subset of the linear solver operations. See the documentation for each SUNDIALS linear solver interface to determine which SUNLINSOL operations they require. 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.
- Optionally, define and implement additional user-callable routines acting on the newly defined `SUNLinearSolver` (e.g., routines to set various configuration options for tuning the linear solver to a particular problem).
- Optionally, provide functions as needed for that particular implementation to access different parts in the *content* field of the newly defined `SUNLinearSolver` object (e.g., routines to return various statistics from the solver).

Each SUNLINSOL implementation included in SUNDIALS has a “type” identifier specified in enumeration and shown in Table 8.1. It is recommended that a user-supplied SUNLINSOL implementation set this identifier based on the SUNDIALS solver interface they intend to use: “Dls” interfaces require the `SUNLINEARSOLVER_DIRECT` SUNLINSOL objects and “Spils” interfaces require the `SUNLINEARSOLVER_ITERATIVE` objects.

Table 8.2: Description of the `SUNLinearSolver` operations

| Name                          | Usage and Description                                                                                                                                                                                                                                                                                                                                                          |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>SUNLinSolGetType</code> | <pre>type = SUNLinSolGetType(LS);</pre> Returns the type identifier for the linear solver <code>LS</code> . It is used to determine the solver type (direct, iterative, or custom) from the abstract <code>SUNLinearSolver</code> interface. This is used to assess compatibility with SUNDIALS-provided linear solver interfaces. Returned values are given in the Table 8.1. |

*continued on next page*

| Name                          | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUNLinSolInitialize           | <pre>ier = SUNLinSolInitialize(LS);</pre> <p>Performs linear solver initialization (assumes that all solver-specific options have been set). 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 8.4.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| SUNLinSolSetup                | <pre>ier = SUNLinSolSetup(LS, A);</pre> <p>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. 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 8.4.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| SUNLinSolSolve                | <pre>ier = SUNLinSolSolve(LS, A, x, b, tol);</pre> <p>Solves a linear system <math>Ax = b</math>. 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 8.4.</p> <p><b>Direct solvers:</b> can ignore the <code>realtype</code> argument <code>tol</code>.</p> <p><b>Iterative solvers:</b> can ignore the SUNMATRIX input A since a NULL argument will be passed (these should instead rely on the matrix-vector product function supplied through the routine SUNLinSolSetATimes). These should attempt to solve to the specified <code>realtype</code> tolerance <code>tol</code> in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.</p> <p><b>Custom solvers:</b> all arguments will be supplied, and if the solver is approximate then it should attempt to solve to the specified <code>realtype</code> tolerance <code>tol</code> in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.</p> |
| SUNLinSolFree                 | <pre>ier = SUNLinSolFree(LS);</pre> <p>Frees memory allocated by the linear solver. This should return zero for a successful call, and a negative value for a failure.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| SUNLinSolSetATimes            | <pre>ier = SUNLinSolSetATimes(LS, A_data, ATimes);</pre> <p>(Iterative/Custom linear solvers only) Provides <code>ATimesFn</code> function pointer, as well as a <code>void *</code> pointer to a data structure used by this routine, to a linear solver object. SUNDIALS solvers 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. 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 8.4.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| <i>continued on next page</i> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |



| Name                          | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUNLinSolSetPreconditioner    | <pre>ier = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);</pre> <p>(Optional; Iterative/Custom linear solvers only) Provides PSetupFn and PSolveFn function pointers that implement the preconditioner solves <math>P_1^{-1}</math> and <math>P_2^{-1}</math> from equations (8.1)-(8.2). This routine will be called by a SUNDIALS solver, which will provide translation between the generic Pset and Psol calls and the integrator-specific and integrator- or user-supplied routines. 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 8.4.</p>                                                                                     |
| SUNLinSolSetScalingVectors    | <pre>ier = SUNLinSolSetScalingVectors(LS, s1, s2);</pre> <p>(Optional; Iterative/Custom linear solvers only) Sets pointers to left/right scaling vectors for the linear system solve. Here, s1 is an NVECTOR of positive scale factors containing the diagonal of the matrix <math>S_1</math> from equations (8.1)-(8.2). Similarly, s2 is an NVECTOR containing the diagonal of <math>S_2</math> from equations (8.1)-(8.2). Neither of these vectors are tested for positivity, and a NULL argument for either indicates that the corresponding scaling matrix is the identity. 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 8.4.</p> |
| SUNLinSolNumIters             | <pre>its = SUNLinSolNumIters(LS);</pre> <p>(Optional; Iterative/Custom linear solvers only) Should return the int number of linear iterations performed in the last ‘solve’ call.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| SUNLinSolResNorm              | <pre>rnorm = SUNLinSolResNorm(LS);</pre> <p>(Optional; Iterative/Custom linear solvers only) Should return the realtype final residual norm from the last ‘solve’ call.</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| SUNLinSolResid                | <pre>rvec = SUNLinSolResid(LS);</pre> <p>(Optional; Iterative/Custom linear solvers only) 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 function may be called by the SUNDIALS solver. This routine should return the NVECTOR containing the preconditioned initial residual vector.</p>                                                                                                                                                                                                                                                                         |
| <i>continued on next page</i> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |

| Name           | Usage and Description                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| SUNLinLastFlag | <code>lflag = SUNLinLastFlag(LS);</code><br>(Optional) Should return the last error flag encountered within the linear solver. This is not called by the SUNDIALS solvers directly; it allows the user to investigate linear solver issues after a failed solve.                                                                                                                                                                                                                            |
| SUNLinSolSpace | <code>ier = SUNLinSolSpace(LS, &amp;lrw, &amp;liw);</code><br>(Optional) Returns the storage requirements for the linear solver LS. <code>lrw</code> is a <code>long int</code> containing the number of realtype words and <code>liw</code> is a <code>long int</code> containing the number of integer words. The return value is an integer flag denoting success/failure of the operation.<br>This function is advisory only, for use in determining a user's total space requirements. |

## 8.1 Description of the client-supplied SUNLinearSolver routines

The SUNDIALS packages provide the `ATimes`, `Pset` and `Psol` routines utilized by the SUNLINSOL modules. These function types are defined in the header file `sundials/sundials_iterative.h`, and are described here in case a user wishes to interact directly with an iterative SUNLINSOL object.

### 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.

**Notes**

### 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.

**Notes**

## PSolveFn

[illegible]

**Purpose** These functions solve the preconditioner equation  $Pz = r$  for the vector  $z$ . Memory for  $\mathbf{z}$  should already be allocated prior to calling this function. The parameter `P_data` is a pointer to any information about  $P$  which the function needs in order to do its job (set up by the corresponding `PSetupFn`). The parameter `lr` is input, and indicates whether  $P$  is to be taken as the left preconditioner or the right preconditioner: `lr = 1` for left and `lr = 2` for right. If preconditioning is on one side only, `lr` can be ignored. If the preconditioner is iterative, then it should strive to solve the preconditioner equation so that

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

where the weight vector for the WRMS norm may be accessed from the main package memory structure. The vector `r` should not be modified by the `PSolveFn`.

Arguments    `P_data` is a pointer to client data, the same pointer as that supplied to the routine `SUNLinSolSetPreconditioner`.

$\mathbf{r}$  is the right-hand side vector for the preconditioner system

$\mathbf{z}$  is the solution vector for the preconditioner system

tol is the desired tolerance for an iterative preconditioner

`lr` is flag indicating whether the routine should perform left (1) or right (2) preconditioning.

**Return value** This routine should return 0 if successful and a non-zero value if unsuccessful. On a failure, a negative return value indicates an unrecoverable condition, while a positive value indicates a recoverable one, in which the calling routine may reattempt the solution after updating preconditioner data.

## Notes

## 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 8.3 we show the direct 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 8.3: SUNDIALS direct linear solvers and matrix implementations that can be used for each.

| Linear Solver Interface | Dense Matrix | Banded Matrix | Sparse Matrix | User Supplied |
|-------------------------|--------------|---------------|---------------|---------------|
| Dense                   | ✓            |               |               | ✓             |
| Band                    |              | ✓             |               | ✓             |
| LapackDense             | ✓            |               |               | ✓             |
| LapackBand              |              | ✓             |               | ✓             |
| KLU                     |              |               | ✓             | ✓             |
| SUPERLUMT               |              |               | ✓             | ✓             |

*continued on next page*

|                         |              |               |               |               |
|-------------------------|--------------|---------------|---------------|---------------|
| Linear Solver Interface | Dense Matrix | Banded Matrix | Sparse Matrix | User Supplied |
| User supplied           | ✓            | ✓             | ✓             | ✓             |

The functions within the SUNDIALS-provided `SUNLinearSolver` implementations return a common set of error codes, shown below in the Table 8.4.

Table 8.4: Description of the `SUNLinearSolver` error codes

| Name                                  | Value | Description                                                                                                                  |
|---------------------------------------|-------|------------------------------------------------------------------------------------------------------------------------------|
| <code>SUNLS_SUCCESS</code>            | 0     | successful call or converged solve                                                                                           |
| <code>SUNLS_MEM_NULL</code>           | -1    | the memory argument to the function is <code>NULL</code>                                                                     |
| <code>SUNLS_ILL_INPUT</code>          | -2    | an illegal input has been provided to the function                                                                           |
| <code>SUNLS_MEM_FAIL</code>           | -3    | failed memory access or allocation                                                                                           |
| <code>SUNLS_ATHES_FAIL_UNREC</code>   | -4    | an unrecoverable failure occurred in the <code>ATHes</code> routine                                                          |
| <code>SUNLS_PSET_FAIL_UNREC</code>    | -5    | an unrecoverable failure occurred in the <code>Pset</code> routine                                                           |
| <code>SUNLS_PSOLVE_FAIL_UNREC</code>  | -6    | an unrecoverable failure occurred in the <code>Psolve</code> routine                                                         |
| <code>SUNLS_PACKAGE_FAIL_UNREC</code> | -7    | an unrecoverable failure occurred in an external linear solver package                                                       |
| <code>SUNLS_GS_FAIL</code>            | -8    | a failure occurred during Gram-Schmidt orthogonalization ( <code>SUNLINSOL_SPGMR</code> / <code>SUNLINSOL_SPFGMR</code> )    |
| <code>SUNLS_QRSOL_FAIL</code>         | -9    | a singular $R$ matrix was encountered in a QR factorization ( <code>SUNLINSOL_SPGMR</code> / <code>SUNLINSOL_SPFGMR</code> ) |
| <code>SUNLS_RES_REDUCED</code>        | 1     | an iterative solver reduced the residual, but did not converge to the desired tolerance                                      |
| <code>SUNLS_CONV_FAIL</code>          | 2     | an iterative solver did not converge (and the residual was not reduced)                                                      |
| <code>SUNLS_ATHES_FAIL_REC</code>     | 3     | a recoverable failure occurred in the <code>ATHes</code> routine                                                             |
| <code>SUNLS_PSET_FAIL_REC</code>      | 4     | a recoverable failure occurred in the <code>Pset</code> routine                                                              |
| <code>SUNLS_PSOLVE_FAIL_REC</code>    | 5     | a recoverable failure occurred in the <code>Psolve</code> routine                                                            |
| <code>SUNLS_PACKAGE_FAIL_REC</code>   | 6     | a recoverable failure occurred in an external linear solver package                                                          |
| <code>SUNLS_QRFACT_FAIL</code>        | 7     | a singular matrix was encountered during a QR factorization ( <code>SUNLINSOL_SPGMR</code> / <code>SUNLINSOL_SPFGMR</code> ) |
| <code>SUNLS_LUFACT_FAIL</code>        | 8     | a singular matrix was encountered during a LU factorization ( <code>SUNLINSOL_DENSE</code> / <code>SUNLINSOL_BAND</code> )   |

### 8.3 The `SUNLinearSolver_Dense` implementation

The dense implementation of the `SUNLINSOL` module provided with SUNDIALS, `SUNLINSOL_DENSE`, 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`). The `SUNLINSOL_DENSE` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Dense {
    sunindextype N;
    sunindextype *pivots;
```

```
    long int last_flag;
};
```

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

**N** - size of the linear system,

**pivots** - index array for partial pivoting in LU factorization,

**last\_flag** - last error return flag from internal function evaluations.

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).

The header file to include when using this module is `sunlinsol/sunlinsol_dense.h`. The SUNLINSOL\_DENSE module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsoldense` module library.

The SUNLINSOL\_DENSE module defines dense implementations of all “direct” linear solver operations listed in Table 8.2:

- `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`

The module SUNLINSOL\_DENSE provides the following additional user-callable constructor routine:

- `SUNDenseLinearSolver`

This function creates and allocates memory for a dense `SUNLinearSolver`. Its arguments are an `NVECTOR` and `SUNMATRIX`, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

This routine will perform consistency checks to ensure that it is called with consistent `NVECTOR` and `SUNMATRIX` implementations. These are currently limited to the `SUNMATRIX_DENSE` matrix type and the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

If either **A** or **y** are incompatible then this routine will return `NULL`.

```
SUNLinearSolver SUNDenseLinearSolver(N_Vector y, SUNMatrix A);
```

For solvers that include a Fortran interface module, the SUNLINSOL\_DENSE module also includes the Fortran-callable function `FSUNDenseLinSolInit(code, ier)` to initialize this SUNLINSOL\_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); `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`. 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 Fortran-callable function `FSUNMassDenseLinSolInit(ier)` initializes this SUNLINSOL\_DENSE module for solving mass matrix linear systems.

## 8.4 The SUNLinearSolver\_Band implementation

The band implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL\_BAND, 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). The SUNLINSOL\_BAND module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Band {
    sunindextype N;
    sunindextype *pivots;
    long int last_flag;
};
```


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

**N** - size of the linear system,

**pivots** - index array for partial pivoting in LU factorization,

**last\_flag** - last error return flag from internal function evaluations.

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  $smu = \text{MIN}(N-1, mu+m1)$ . The lower triangular factor  $L$  has lower bandwidth **m1**.

The header file to include when using this module is `sunlinsol/sunlinsol.band.h`. The SUNLINSOL\_BAND module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolband` module library.

The SUNLINSOL\_BAND module defines band implementations of all “direct” linear solver operations listed in Table 8.2:

- `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`

The module `SUNLINSOL_BAND` provides the following additional user-callable constructor routine:

- `SUNBandLinearSolver`

This function creates and allocates memory for a band `SUNLinearSolver`. Its arguments are an `NVECTOR` and `SUNMATRIX`, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

This routine will perform consistency checks to ensure that it is called with consistent `NVECTOR` and `SUNMATRIX` implementations. These are currently limited to the `SUNMATRIX_BAND` matrix type and the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector types. As additional compatible matrix and vector implementations are added to `SUNDIALS`, these will be included within this compatibility check.

Additionally, this routine will verify that the input matrix `A` is allocated with appropriate upper bandwidth storage for the *LU* factorization.

If either `A` or `y` are incompatible then this routine will return `NULL`.

```
SUNLinearSolver SUNBandLinearSolver(N_Vector y, SUNMatrix A);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_BAND` module also includes the Fortran-callable function `FSUNBandLinSolInit(code, ier)` to initialize this `SUNLINSOL_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`); `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`. 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 Fortran-callable function `FSUNMassBandLinSolInit(ier)` initializes this `SUNLINSOL_BAND` module for solving mass matrix linear systems.

## 8.5 The SUNLinearSolver\_LapackDense implementation

The LAPACK dense implementation of the `SUNLINSOL` module provided with `SUNDIALS`, `SUNLINSOL_LAPACKDENSE`, 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`). The `SUNLINSOL_LAPACKDENSE` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Dense {
    sunindextype N;
    sunindextype *pivots;
    long int last_flag;
};
```

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

`N` - size of the linear system,

`pivots` - index array for partial pivoting in *LU* factorization,

`last_flag` - last error return flag from internal function evaluations.



The `SUNLINSOL_LAPACKDENSE` module is a `SUNLINSOL` wrapper for the LAPACK dense matrix factorization and solve routines, `*GETRF` and `*GETRS`, where `*` is either `D` or `S`, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see Section 4.2). In order to use the `SUNLINSOL_LAPACKDENSE` module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see Appendix A for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the `SUNLINSOL_LAPACKDENSE` module also cannot be compiled when using `int64.t` for the `sunindextype`.

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).

The header file to include when using this module is `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 defines dense implementations of all “direct” linear solver operations listed in Table 8.2:

- `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`

The module `SUNLINSOL_LAPACKDENSE` provides the following additional user-callable constructor routine:

- `SUNLapackDense`

This function creates and allocates memory for a LAPACK dense `SUNLinearSolver`. Its arguments are an `NVECTOR` and `SUNMATRIX`, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

This routine will perform consistency checks to ensure that it is called with consistent `NVECTOR` and `SUNMATRIX` implementations. These are currently limited to the `SUNMATRIX_DENSE` matrix type and the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

If either  $A$  or  $y$  are incompatible then this routine will return `NULL`.

`SUNLinearSolver SUNLapackDense(N_Vector y, SUNMatrix A);`



For solvers that include a Fortran interface module, the SUNLINSOL\_LAPACKDENSE module also includes the Fortran-callable function `FSUNLapackDenseInit(code, ier)` to initialize this SUNLINSOL\_LAPACKDENSE 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); `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`. 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 Fortran-callable function `FSUNMassLapackDenseInit(ier)` initializes this SUNLINSOL\_LAPACKDENSE module for solving mass matrix linear systems.

## 8.6 The SUNLinearSolver\_LapackBand implementation

The LAPACK band implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL\_LAPACKBAND, 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). The SUNLINSOL\_LAPACKBAND module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_Band {
    sunindextype N;
    sunindextype *pivots;
    long int last_flag;
};
```

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

**N** - size of the linear system,

**pivots** - index array for partial pivoting in LU factorization,

**last\_flag** - last error return flag from internal function evaluations.

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 `int64_t` for the `sunindextype`.

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`.



The header file to include when using this module is `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 defines band implementations of all “direct” linear solver operations listed in Table 8.2:

- `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`

The module `SUNLINSOL_LAPACKBAND` provides the following additional user-callable routine:

- `SUNLapackBand`

This function creates and allocates memory for a LAPACK band `SUNLinearSolver`. Its arguments are an `NVECTOR` and `SUNMATRIX`, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

This routine will perform consistency checks to ensure that it is called with consistent `NVECTOR` and `SUNMATRIX` implementations. These are currently limited to the `SUNMATRIX_BAND` matrix type and the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector types. As additional compatible matrix and vector implementations are added to `SUNDIALS`, these will be included within this compatibility check.

Additionally, this routine will verify that the input matrix `A` is allocated with appropriate upper bandwidth storage for the  $LU$  factorization.

If either `A` or `y` are incompatible then this routine will return `NULL`.

```
SUNLinearSolver SUNLapackBand(N_Vector y, SUNMatrix A);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_LAPACKBAND` module also includes the Fortran-callable function `FSUNLapackBandInit(code, ier)` to initialize this `SUNLINSOL_LAPACKBAND` 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`); `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`. 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 Fortran-callable function `FSUNMassLapackBandInit(ier)` initializes this `SUNLINSOL_LAPACKBAND` module for solving mass matrix linear systems.

## 8.7 The SUNLinearSolver\_KLU implementation

The `KLU` implementation of the `SUNLINSOL` module provided with `SUNDIALS`, `SUNLINSOL_KLU`, 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 `SUNLINSOL_KLU` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```

struct _SUNLinearSolverContent_KLU {
    long int      last_flag;
    int           first_factorize;
    sun_klu_symbolic *symbolic;
    sun_klu_numeric *numeric;
    sun_klu_common common;
    sunindextype  (*klu_solver)(sun_klu_symbolic*, sun_klu_numeric*,
                                sunindextype, sunindextype,
                                double*, sun_klu_common*);
};

```

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

**last\_flag** - last error return flag from internal function evaluations,

**first\_factorize** - flag indicating whether the factorization has ever been performed,

**symbolic** - KLU storage structure for symbolic factorization components,

**numeric** - KLU storage structure for numeric factorization components,

**common** - storage structure for common KLU solver components,

**klu\_solver** – pointer to the appropriate KLU solver function (depending on whether it is using a CSR or CSC sparse matrix).

The SUNLINSOL\_KLU module is a SUNLINSOL wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis [1, 14]. In order to use the SUNLINSOL\_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see Appendix A for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have **realtype** set to either **extended** or **single** (see Section 4.2). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available **sunindextype** options.

The KLU library has a symbolic factorization routine that computes the permutation of the linear system matrix to block triangular form and the permutations that will pre-order the diagonal blocks (the only ones that need to be factored) to reduce fill-in (using AMD, COLAMD, CHOLAMD, natural, or an ordering given by the user). Of these ordering choices, the default value in the SUNLINSOL\_KLU module is the COLAMD ordering.

KLU breaks the factorization into two separate parts. The first is a symbolic factorization and the second is a numeric factorization that returns the factored matrix along with final pivot information. KLU also has a refactor routine that can be called instead of the numeric factorization. This routine will reuse the pivot information. This routine also returns diagnostic information that a user can examine to determine if numerical stability is being lost and a full numerical factorization should be done instead of the refactor.

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

- The first time that the “setup” routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.
- On subsequent calls to the “setup” routine, it calls the appropriate KLU “refactor” routine, followed by estimates of the numerical conditioning using the relevant “rcond”, and if necessary “condest”, routine(s). If these estimates of the condition number are larger than  $\varepsilon^{-2/3}$  (where  $\varepsilon$  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.

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 defines implementations of all “direct” linear solver operations listed in Table 8.2:

- `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`

The module SUNLINSOL\_KLU provides the following additional user-callable routines:

- `SUNKLU`

This constructor function creates and allocates memory for a SUNLINSOL\_KLU object. Its arguments are an NVECTOR and SUNMATRIX, that it uses to determine the linear system size and to assess compatibility with the linear solver implementation.

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.

If either *A* or *y* are incompatible then this routine will return NULL.

```
SUNLinearSolver SUNKLU(N_Vector y, SUNMatrix A);
```

- `SUNKLUReInit`

This function 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).

The `reinit_type` argument governs the level of reinitialization. The allowed values are:

- `SUNKLU_REINIT_FULL` – The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.
- `SUNKLU_REINIT_PARTIAL` – Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the sparse matrix provided to the original constructor routine (or the previous `SUNKLUReInit` call).

This routine assumes no other changes to solver use are necessary.

The return values from this function are `SUNLS_MEM_NULL` (either `S` or `A` are `NULL`), `SUNLS_ILL_INPUT` (`A` does not have type `SUNMATRIX_SPARSE` or `reinit_type` is invalid), `SUNLS_MEM_FAIL` (reallocation of the sparse matrix failed) or `SUNLS_SUCCESS`.

```
int SUNKLUReInit(SUNLinearSolver S, SUNMatrix A,
                 sunindextype nnz, int reinit_type);
```

- **SUNKLUSetOrdering**

This function sets the ordering used by KLU for reducing fill in the linear solve. Options for `ordering_choice` are:

- 0 AMD,
- 1 COLAMD, and
- 2 the natural ordering.

The default is 1 for COLAMD.

The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid `ordering_choice`), or `SUNLS_SUCCESS`.

```
int SUNKLUSetOrdering(SUNLinearSolver S, int ordering_choice);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_KLU` module also includes the Fortran-callable function `FSUNKLUInit(code, ier)` to initialize this `SUNLINSOL_KLU` 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`); `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`. 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 Fortran-callable function `FSUNMassKLUIInit(ier)` initializes this `SUNLINSOL_KLU` module for solving mass matrix linear systems.

The `SUNKLUReInit` and `SUNKLUSetOrdering` routines also support Fortran interfaces for the system and mass matrix solvers:

- `FSUNKLUReInit(code, NNZ, reinit_type, ier)` – `NNZ` should be commensurate with a C `long int` and `reinit_type` should be commensurate with a C `int` (1 = 'FULL', 2 = 'PARTIAL')
- `FSUNMassKLUReInit(NNZ, reinit_type, ier)`
- `FSUNKLUSetOrdering(code, ordering, ier)` – `ordering` should be commensurate with a C `int`
- `FSUNMassKLUSetOrdering(ordering, ier)`

## 8.8 The SUNLinearSolver\_SuperLUMT implementation

The `SUPERLUMT` implementation of the `SUNLINSOL` module provided with SUNDIALS, `SUNLINSOL_SUPERLUMT`, 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 `SUNLINSOL_SUPERLUMT` module defines the `content` field of a `SUNLinearSolver` to be the following structure:

```

struct _SUNLinearSolverContent_SuperLUMT {
    long int    last_flag;
    int         first_factorize;
    SuperMatrix *A, *AC, *L, *U, *B;
    Gstat_t     *Gstat;
    sunindextype *perm_r, *perm_c;
    sunindextype N;
    int         num_threads;
    realtype     diag_pivot_thresh;
    int         ordering;
    superlumt_options_t *options;
};

```

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

**last\_flag** - last error return flag from internal function evaluations,

**first\_factorize** - flag indicating whether the factorization has ever been performed,

**A, AC, L, U, B** - SuperMatrix pointers used in solve,

**Gstat** - GStat\_t object used in solve,

**perm\_r, perm\_c** - permutation arrays used in solve,

**N** - size of the linear system,

**num\_threads** - number of OpenMP/Pthreads threads to use,

**diag\_pivot\_thresh** - threshold on diagonal pivoting,

**ordering** - flag for which reordering algorithm to use,

**options** - pointer to SUPERLUMT options structure.



The SUNLINSOL\_SUPERLUMT module is a SUNLINSOL wrapper for the SUPERLUMT sparse matrix factorization and solver library written by X. Sherry Li [2, 31, 16]. 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.

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.

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

The SUNLINSOL\_SUPERLUMT module defines implementations of all “direct” linear solver operations listed in Table 8.2:

- `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 module SUNLINSOL\_SUPERLUMT provides the following additional user-callable routines:

- `SUNSuperLUMT`

This constructor function creates and allocates memory for a SUNLINSOL\_SUPERLUMT object. Its arguments are an NVECTOR, a SUNMATRIX, and a desired number of threads (OpenMP or Pthreads, depending on how SUPERLUMT was installed) to use during the factorization steps. This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SUPERLUMT library.

This routine will perform consistency checks to ensure that it is called with consistent NVECTOR and SUNMATRIX implementations. These are currently limited to the SUNMATRIX\_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR\_SERIAL, NVECTOR\_OPENMP, and NVECTOR\_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

If either *A* or *y* are incompatible then this routine will return NULL. The `num_threads` argument is not checked and is passed directly to SUPERLUMT routines.

```
SUNLinearSolver SUNSuperLUMT(N_Vector y, SUNMatrix A, int num_threads);
```

- `SUNSuperLUMTSetOrdering`

This function sets the ordering used by SUPERLUMT for reducing fill in the linear solve. Options for `ordering_choice` 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.

The return values from this function are `SUNLS_MEM_NULL` (`S` is `NULL`), `SUNLS_ILL_INPUT` (invalid `ordering_choice`), or `SUNLS_SUCCESS`.

```
int SUNSuperLUMTSetOrdering(SUNLinearSolver S, int ordering_choice);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_SUPERLUMT` module also includes the Fortran-callable function `FSUNSuperLUMTInit(code, num_threads, ier)` to initialize this `SUNLINSOL_SUPERLUMT` 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`); `num_threads` is the desired number of OpenMP/Pthreads threads to use in the factorization; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these arguments should be declared so as to match C type `int`. 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 Fortran-callable function `FSUNMassSuperLUMTInit(num_threads, ier)` initializes this `SUNLINSOL_SUPERLUMT` module for solving mass matrix linear systems.

The `SUNSuperLUMTSetOrdering` routine also supports Fortran interfaces for the system and mass matrix solvers:

- `FSUNSuperLUMTSetOrdering(code, ordering, ier)` – `ordering` should be commensurate with a C `int`
- `FSUNMassSuperLUMTSetOrdering(ordering, ier)`

## 8.9 The SUNLinearSolver\_SPGMR implementation

The `SPGMR` (Scaled, Preconditioned, Generalized Minimum Residual [36]) implementation of the `SUNLINSOL` module provided with `SUNDIALS`, `SUNLINSOL_SPGMR`, is an iterative linear solver that is designed to be compatible with any `NVECTOR` implementation (serial, threaded, parallel, and user-supplied) that supports a minimal subset of operations (`N_VClone`, `N_VDotProd`, `N_VScale`, `N_VLinearSum`, `N_VProd`, `N_VConst`, `N_VDiv`, and `N_VDestroy`).

The `SUNLINSOL_SPGMR` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPGMR {
    int maxl;
    int pretype;
    int gstype;
    int max_restarts;
    int numiters;
    realtype resnorm;
    long int last_flag;
    ATimesFn ATimes;
    void* ATData;
    PSetupFn Psetup;
    PSolveFn Psolve;
    void* PData;
    N_Vector s1;
    N_Vector s2;
    N_Vector *V;
    realtype **Hes;
    realtype *givens;
    N_Vector xcor;
    realtype *yg;
    N_Vector vtemp;
};
```



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

- maxl** - number of GMRES basis vectors to use (default is 5),
- pretype** - flag for type of preconditioning to employ (default is none),
- gstype** - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),
- max\_restarts** - number of GMRES restarts to allow (default is 0),
- numiters** - number of iterations from the most-recent solve,
- resnorm** - final linear residual norm from the most-recent solve,
- last\_flag** - last error return flag from an internal function,
- ATimes** - function pointer to perform  $Av$  product,
- ATData** - pointer to structure for **ATimes**,
- Psetup** - function pointer to preconditioner setup routine,
- Psolve** - function pointer to preconditioner solve routine,
- PData** - pointer to structure for **Psetup** and **Psolve**,
- s1, s2** - vector pointers for supplied scaling matrices (default is NULL),
- V** - the array of Krylov basis vectors  $v_1, \dots, v_{\max l+1}$ , stored in  $V[0], \dots, V[\max l]$ . Each  $v_i$  is a vector of type NVECTOR.,
- Hes** - the  $(\max l + 1) \times \max l$  Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by  $Hes[i][j]$ .,
- givens** - a length  $2*\max l$  array which represents the Givens rotation matrices that arise in the GMRES

algorithm. These matrices are  $F_0, F_1, \dots, F_j$ , where  $F_i =$

$$\begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c_i & -s_i & & \\ & & & s_i & c_i & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{bmatrix},$$

are represented in the **givens** vector as **givens**[0] =  $c_0$ , **givens**[1] =  $s_0$ , **givens**[2] =  $c_1$ , **givens**[3] =  $s_1$ , ... **givens**[2j] =  $c_j$ , **givens**[2j+1] =  $s_j$ .,

- xcor** - a vector which holds the scaled, preconditioned correction to the initial guess,
- yg** - a length  $(\max l+1)$  array of **realtype** values used to hold “short” vectors (e.g.  $y$  and  $g$ ),
- vtemp** - temporary vector storage.

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.

The header file to include when using this module is `sunlinsol/sunlinsol_spgmr.h`. The `SUNLINSOL_SPGMR` module is accessible from all SUNDIALS solvers *without* linking to the

`libsundials_sunlinsolspgmr` module library.

The `SUNLINSOL_SPGMR` module defines implementations of all “iterative” linear solver operations listed in Table 8.2:

- `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`

The module `SUNLINSOL_SPGMR` provides the following additional user-callable routines:

- `SUNSPGMR`

This constructor function creates and allocates memory for a `SPGMR SUNLinearSolver`. Its arguments are an `NVECTOR`, the desired type of preconditioning, and the number of Krylov basis vectors to use.

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`.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

Allowable inputs for `pretype` are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3); any other integer input will result in the default (no preconditioning). 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.

```
SUNLinearSolver SUNSPGMR(N_Vector y, int pretype, int maxl);
```

- **SUNSPGMRSetPrecType**

This function updates the type of preconditioning to use. Supported values are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3).

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNSPGMRSetPrecType(SUNLinearSolver S, int pretype);
```

- **SUNSPGMRSetGSType**

This function sets the type of Gram-Schmidt orthogonalization to use. Supported values are `MODIFIED_GS` (1) and `CLASSICAL_GS` (2). Any other integer input will result in a failure, returning error code `SUNLS_ILL_INPUT`.

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `gstype`), `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNSPGMRSetGSType(SUNLinearSolver S, int gstype);
```

- **SUNSPGMRSetMaxRestarts**

This function sets the number of GMRES restarts to allow. A negative input will result in the default of 0.

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNSPGMRSetMaxRestarts(SUNLinearSolver S, int maxrs);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_SPGMR` module also includes the Fortran-callable function `FSUNSPGMRInit(code, pretype, maxl, ier)` to initialize this `SUNLINSOL_SPGMR` 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`); `pretype` and `maxl` are the same as for the C function `SUNSPGMR`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the `NVECTOR` object has been initialized. Additionally, when using `ARKODE` with a non-identity mass matrix, the Fortran-callable function `FSUNMassSPGMRInit(pretype, maxl, ier)` initializes this `SUNLINSOL_SPGMR` module for solving mass matrix linear systems.

The `SUNSPGMRSetPrecType`, `SUNSPGMRSetGSType` and `SUNSPGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPGMRSetGSType(code, gstype, ier)`
- `FSUNMassSPGMRSetGSType(gstype, ier)`
- `FSUNSPGMRSetPrecType(code, pretype, ier)`
- `FSUNMassSPGMRSetPrecType(pretype, ier)`
- `FSUNSPGMRSetMaxRS(code, maxrs, ier)`
- `FSUNMassSPGMRSetMaxRS(maxrs, ier)`

## 8.10 The SUNLinearSolver\_SPFGMR implementation

The SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [35]) implementation of the `SUNLINSOL` module provided with SUNDIALS, `SUNLINSOL_SPFGMR`, is an iterative linear solver that is designed to be compatible with any `NVECTOR` implementation (serial, threaded, parallel, and user-supplied) 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 other Krylov iterative linear

solvers supplied with SUNDIALS, FGMRES is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

The SUNLINSOL\_SPFGMR module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPFGMR {
    int maxl;
    int pretype;
    int gstype;
    int max_restarts;
    int numiters;
    realtype resnorm;
    long int last_flag;
    ATimesFn ATimes;
    void* ATData;
    PSetupFn Psetup;
    PSolveFn Psolve;
    void* PData;
    N_Vector s1;
    N_Vector s2;
    N_Vector *V;
    N_Vector *Z;
    realtype **Hes;
    realtype *givens;
    N_Vector xcor;
    realtype *yg;
    N_Vector vtemp;
};
```

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

**maxl** - number of FGMRES basis vectors to use (default is 5),

**pretype** - flag for use of preconditioning (default is none),

**gstype** - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

**max\_restarts** - number of FGMRES restarts to allow (default is 0),

**numiters** - number of iterations from the most-recent solve,

**resnorm** - final linear residual norm from the most-recent solve,

**last\_flag** - last error return flag from an internal function,

**ATimes** - function pointer to perform  $Av$  product,

**ATData** - pointer to structure for **ATimes**,

**Psetup** - function pointer to preconditioner setup routine,

**Psolve** - function pointer to preconditioner solve routine,

**PData** - pointer to structure for **Psetup** and **Psolve**,

**s1**, **s2** - vector pointers for supplied scaling matrices (default is NULL),

**V** - the array of Krylov basis vectors  $v_1, \dots, v_{\text{maxl}+1}$ , stored in  $V[0], \dots, V[\text{maxl}]$ . Each  $v_i$  is a vector of type `NVECTOR`.,

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

**Hes** - the  $(\text{maxl} + 1) \times \text{maxl}$  Hessenberg matrix. It is stored row-wise so that the  $(i,j)$ th element is given by `Hes[i][j]`.,

**givens** - a length  $2 \times \text{maxl}$  array which represents the Givens rotation matrices that arise in the FGM-

RES algorithm. These matrices are  $F_0, F_1, \dots, F_j$ , where  $F_i =$

$$\begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c_i & -s_i & & \\ & & & s_i & c_i & & \\ & & & & & 1 & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix},$$

are represented in the **givens** vector as `givens[0] =  $c_0$` , `givens[1] =  $s_0$` , `givens[2] =  $c_1$` , `givens[3] =  $s_1$` , ... `givens[2j] =  $c_j$` , `givens[2j+1] =  $s_j$` .,

**xcor** - a vector which holds the scaled, preconditioned correction to the initial guess,

**yg** - a length  $(\text{maxl}+1)$  array of `realtype` values used to hold “short” vectors (e.g.  $y$  and  $g$ ),

**vtemp** - temporary vector storage.

This solver is constructed to perform the following operations:

- During construction, the **xcor** and **vtemp** arrays are cloned from a template `NVECTOR` that is input, and default solver parameters are set.
- User-facing “set” routines may be called to modify default solver parameters.
- Additional “set” routines are called by the SUNDIALS solver that interfaces with `SUNLINSOL_SPFGMR` to supply the **ATimes**, **PSetup**, and **Psolve** function pointers and **s1** and **s2** scaling vectors.
- In the “initialize” call, the remaining solver data is allocated (**V**, **Hes**, **givens**, and **yg** )
- In the “setup” call, any non-NULL **PSetup** function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic **PSetup** function and the solver-specific routine (solver-supplied or user-supplied).
- In the “solve” call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

The header file to include when using this module is `sunlinsol/sunlinsol_spfgmr.h`. The `SUNLINSOL_SPFGMR` module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolspfgmr` module library.

The `SUNLINSOL_SPFGMR` module defines implementations of all “iterative” linear solver operations listed in Table 8.2:

- `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`

The module `SUNLINSOL_SPFGMR` provides the following additional user-callable routines:

- `SUNSPFGMR`

This constructor function creates and allocates memory for a SPFGMR `SUNLinearSolver`. Its arguments are an `NVECTOR`, a flag indicating to use preconditioning, and the number of Krylov basis vectors to use.

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`.

A `max1` argument that is  $\leq 0$  will result in the default value (5).

Since the FGMRES algorithm is designed to only support right preconditioning, then any of the `pretype` inputs `PREC_LEFT` (1), `PREC_RIGHT` (2), or `PREC_BOTH` (3) will result in use of `PREC_RIGHT`; any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS). While it is possible to use a right-preconditioned `SUNLINSOL_SPFGMR` object for these packages, this use mode is not supported and may result in inferior performance.

`SUNLinearSolver SUNSPFGMR(N_Vector y, int pretype, int max1);`

- `SUNSPFGMRSetPrecType`

This function updates the flag indicating use of preconditioning. Since the FGMRES algorithm is designed to only support right preconditioning, then any of the `pretype` inputs `PREC_LEFT` (1), `PREC_RIGHT` (2), or `PREC_BOTH` (3) will result in use of `PREC_RIGHT`; any other integer input will result in the default (no preconditioning).

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

`int SUNSPFGMRSetPrecType(SUNLinearSolver S, int pretype);`

- `SUNSPFGMRSetGSType`

This function sets the type of Gram-Schmidt orthogonalization to use. Supported values are `MODIFIED_GS` (1) and `CLASSICAL_GS` (2). Any other integer input will result in a failure, returning error code `SUNLS_ILL_INPUT`.

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `gstype`), `SUNLS_MEM_NULL` (`S` is `NULL`), or `SUNLS_SUCCESS`.

`int SUNSPFGMRSetGSType(SUNLinearSolver S, int gstype);`

- `SUNSPFGMRSetMaxRestarts`

This function sets the number of FGMRES restarts to allow. A negative input will result in the default of 0.

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

`int SUNSPFGMRSetMaxRestarts(SUNLinearSolver S, int maxrs);`

For solvers that include a Fortran interface module, the SUNLINSOL\_SPFGMR module also includes the Fortran-callable function `FSUNSPFGMRInit(code, pretype, maxl, ier)` to initialize this SUNLINSOL\_SPFGMR 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); `pretype` and `maxl` are the same as for the C function `SUNSPFGMR`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the `NVECTOR` object has been initialized. Additionally, when using ARKODE with a non-identity mass matrix, the Fortran-callable function `FSUNMassSPFGMRInit(pretype, maxl, ier)` initializes this SUNLINSOL\_SPFGMR module for solving mass matrix linear systems.

The `SUNSPFGMRSetPrecType`, `SUNSPFGMRSetGStype`, and `SUNSPFGMRSetMaxRestarts` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPFGMRSetGStype(code, gstype, ier)`
- `FSUNMassSPFGMRSetGStype(gstype, ier)`
- `FSUNSPFGMRSetPrecType(code, pretype, ier)`
- `FSUNMassSPFGMRSetPrecType(pretype, ier)`
- `FSUNSPFGMRSetMaxRS(code, maxrs, ier)`
- `FSUNMassSPFGMRSetMaxRS(maxrs, ier)`

## 8.11 The SUNLinearSolver\_SPBCGS implementation

The SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [37]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL\_SPBCGS, is an iterative linear solver that is designed to be compatible with any `NVECTOR` implementation (serial, threaded, parallel, and user-supplied) 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.

The SUNLINSOL\_SPBCGS module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPBCGS {
    int maxl;
    int pretype;
    int numiters;
    realtype resnorm;
    long int last_flag;
    ATimesFn ATimes;
    void* ATData;
    PSetupFn Psetup;
    PSolveFn Psolve;
    void* PData;
    N_Vector s1;
    N_Vector s2;
    N_Vector r;
    N_Vector r_star;
    N_Vector p;
    N_Vector q;
    N_Vector u;
    N_Vector Ap;
    N_Vector vtemp;
};
```

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

**maxl** - number of SPBCGS iterations to allow (default is 5),  
**pretype** - flag for type of preconditioning to employ (default is none),  
**numiters** - number of iterations from the most-recent solve,  
**resnorm** - final linear residual norm from the most-recent solve,  
**last\_flag** - last error return flag from an internal function,  
**ATimes** - function pointer to perform  $Av$  product,  
**ATData** - pointer to structure for **ATimes**,  
**Psetup** - function pointer to preconditioner setup routine,  
**Psolve** - function pointer to preconditioner solve routine,  
**PData** - pointer to structure for **Psetup** and **Psolve**,  
**s1, s2** - vector pointers for supplied scaling matrices (default is NULL),  
**r** - a NVECTOR which holds the current scaled, preconditioned linear system residual,  
**r\_star** - a NVECTOR which holds the initial scaled, preconditioned linear system residual,  
**p, q, u, Ap, vtemp** - NVECTORS used for workspace by the SPBCGS algorithm.

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.

The header file to include when using this module is `sunlinsol/sunlinsol.spbcgs.h`. The SUNLINSOL\_SPBCGS module is accessible from all SUNDIALS solvers *without* linking to the `libsundials.sunlinsolspbcgs` module library.

The SUNLINSOL\_SPBCGS module defines implementations of all “iterative” linear solver operations listed in Table 8.2:

- `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

The module SUNLINSOL\_SPBCGS provides the following additional user-callable routines:

- SUNSPBCGS

This constructor function creates and allocates memory for a SPBCGS `SUNLinearSolver`. Its arguments are an `NVECTOR`, the desired type of preconditioning, and the number of linear iterations to allow.

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`.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

Allowable inputs for `pretype` are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3); any other integer input will result in the default (no preconditioning). 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.

```
SUNLinearSolver SUNSPBCGS(N_Vector y, int pretype, int maxl);
```

- SUNSPBCGSSetPrecType

This function updates the type of preconditioning to use. Supported values are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2), and `PREC_BOTH` (3).

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`), or `SUNLS_SUCCESS`.

```
int SUNSPBCGSSetPrecType(SUNLinearSolver S, int pretype);
```

- SUNSPBCGSSetMaxl

This function updates the number of linear solver iterations to allow.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNSPBCGSSetMaxl(SUNLinearSolver S, int maxl);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_SPBCGS` module also includes the Fortran-callable function `FSUNSPBCGSInit(code, pretype, maxl, ier)` to initialize this `SUNLINSOL_SPBCGS` 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`); `pretype` and `maxl` are the same as for the C function `SUNSPBCGS`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the `NVECTOR` object has been initialized. Additionally, when using `ARKODE` with a non-identity

mass matrix, the Fortran-callable function `FSUNMassSPBCGSInit(pretype, maxl, ier)` initializes this `SUNLINSOL_SPBCGS` module for solving mass matrix linear systems.

The `SUNSPBCGSSetPrecType` and `SUNSPBCGSsetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPBCGSSetPrecType(code, pretype, ier)`
- `FSUNMassSPBCGSSetPrecType(pretype, ier)`
- `FSUNSPBCGSsetMaxl(code, maxl, ier)`
- `FSUNMassSPBCGSsetMaxl(maxl, ier)`

## 8.12 The SUNLinearSolver\_SPTFQMR implementation

The SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [19]) implementation of the `SUNLINSOL` module provided with `SUNDIALS`, `SUNLINSOL_SPTFQMR`, is an iterative linear solver that is designed to be compatible with any `NVECTOR` implementation (serial, threaded, parallel, and user-supplied) 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.

The `SUNLINSOL_SPTFQMR` module defines the *content* field of a `SUNLinearSolver` to be the following structure:

```
struct _SUNLinearSolverContent_SPTFQMR {
    int maxl;
    int pretype;
    int numiters;
    realtype resnorm;
    long int last_flag;
    ATimesFn ATimes;
    void* ATData;
    PSetupFn Psetup;
    PSolveFn Psolve;
    void* PData;
    N_Vector s1;
    N_Vector s2;
    N_Vector r_star;
    N_Vector q;
    N_Vector d;
    N_Vector v;
    N_Vector p;
    N_Vector *r;
    N_Vector u;
    N_Vector vtemp1;
    N_Vector vtemp2;
    N_Vector vtemp3;
};
```

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

**maxl** - number of TFQMR iterations to allow (default is 5),

**pretype** - flag for type of preconditioning to employ (default is none),

**numiters** - number of iterations from the most-recent solve,

**resnorm** - final linear residual norm from the most-recent solve,  
**last\_flag** - last error return flag from an internal function,  
**ATimes** - function pointer to perform  $Av$  product,  
**ATData** - pointer to structure for **ATimes**,  
**Psetup** - function pointer to preconditioner setup routine,  
**Psolve** - function pointer to preconditioner solve routine,  
**PData** - pointer to structure for **Psetup** and **Psolve**,  
**s1, s2** - vector pointers for supplied scaling matrices (default is NULL),  
**r\_star** - a NVECTOR which holds the initial scaled, preconditioned linear system residual,  
**q, d, v, p, u** - NVECTORS used for workspace by the SPTFQMR algorithm,  
**r** - array of two NVECTORS used for workspace within the SPTFQMR algorithm,  
**vtemp1, vtemp2, vtemp3** - temporary vector storage.

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.

The header file to include when using this module is `sunlinsol/sunlinsol.sptfqmr.h`. The SUNLINSOL\_SPTFQMR module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolsptfqmr` module library.

The SUNLINSOL\_SPTFQMR module defines implementations of all “iterative” linear solver operations listed in Table 8.2:

- `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

The module SUNLINSOL\_SPTFQMR provides the following additional user-callable routines:

- SUNSPTFQMR

This constructor function creates and allocates memory for a SPTFQMR `SUNLinearSolver`. Its arguments are an `NVECTOR`, the desired type of preconditioning, and the number of linear iterations to allow.

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`.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

Allowable inputs for `pretype` are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2) and `PREC_BOTH` (3); any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a `SUNLINSOL_SPTFQMR` object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

```
SUNLinearSolver SUNSPTFQMR(N_Vector y, int pretype, int maxl);
```

- SUNSPTFQMRSetPrecType

This function updates the type of preconditioning to use. Supported values are `PREC_NONE` (0), `PREC_LEFT` (1), `PREC_RIGHT` (2), and `PREC_BOTH` (3).

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`), or `SUNLS_SUCCESS`.

```
int SUNSPTFQMRSetPrecType(SUNLinearSolver S, int pretype);
```

- SUNSPTFQMRSetMaxl

This function updates the number of linear solver iterations to allow.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNSPTFQMRSetMaxl(SUNLinearSolver S, int maxl);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_SPTFQMR` module also includes the Fortran-callable function `FSUNSPTFQMRInit(code, pretype, maxl, ier)` to initialize this `SUNLINSOL_SPTFQMR` 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`); `pretype` and `maxl` are the same as for the C function `SUNSPTFQMR`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the `NVECTOR` object has been initialized. Additionally, when using `ARKODE` with a non-identity mass matrix, the Fortran-callable function `FSUNMassSPTFQMRInit(pretype, maxl, ier)` initializes this `SUNLINSOL_SPTFQMR` module for solving mass matrix linear systems.

The `SUNSPTFQMRSetPrecType` and `SUNSPTFQMRSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNSPTFQMRSetPrecType(code, pretype, ier)`

- FSUNMassSPTFQMRSetPrecType(precType, ier)
- FSUNSPTFQMRSetMaxl(code, maxl, ier)
- FSUNMassSPTFQMRSetMaxl(maxl, ier)

## 8.13 The SUNLinearSolver\_PCG implementation

The PCG (Preconditioned Conjugate Gradient [20]) implementation of the SUNLINSOL module provided with SUNDIALS, SUNLINSOL\_PCG, is an iterative linear solver that is designed to be compatible with any NVECTOR implementation (serial, threaded, parallel, and user-supplied) 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.

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

$$\tilde{A}\tilde{x} = \tilde{b} \quad (8.3)$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \quad (8.4)$$

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  $\delta$ .

The SUNLINSOL\_PCG module defines the *content* field of a SUNLinearSolver to be the following structure:

```
struct _SUNLinearSolverContent_PCG {
    int maxl;
    int pretype;
```

```

    int numiters;
    realtype resnorm;
    long int last_flag;
    ATimesFn ATimes;
    void* ATData;
    PSetupFn Psetup;
    PSolveFn Psolve;
    void* PData;
    N_Vector s;
    N_Vector r;
    N_Vector p;
    N_Vector z;
    N_Vector Ap;
};

```

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

**maxl** - number of PCG iterations to allow (default is 5),

**pretype** - flag for use of preconditioning (default is none),

**numiters** - number of iterations from the most-recent solve,

**resnorm** - final linear residual norm from the most-recent solve,

**last\_flag** - last error return flag from an internal function,

**ATimes** - function pointer to perform  $Av$  product,

**ATData** - pointer to structure for **ATimes**,

**Psetup** - function pointer to preconditioner setup routine,

**Psolve** - function pointer to preconditioner solve routine,

**PData** - pointer to structure for **Psetup** and **Psolve**,

**s** - vector pointer for supplied scaling matrix (default is **NULL**),

**r** - a **NVECTOR** which holds the preconditioned linear system residual,

**p**, **z**, **Ap** - **NVECTORS** used for workspace by the PCG algorithm.

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.

The header file to include when using this module is `sunlinsol/sunlinsol_pcg.h`. The SUNLINSOL\_PCG module is accessible from all SUNDIALS solvers *without* linking to the

`libsundials_sunlinsolpcg` module library.

The SUNLINSOL\_PCG module defines implementations of all “iterative” linear solver operations listed in Table 8.2:

- `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`

The module SUNLINSOL\_PCG provides the following additional user-callable routines:

- `SUNPCG`

This constructor function creates and allocates memory for a PCG `SUNLinearSolver`. Its arguments are an `NVECTOR`, a flag indicating to use preconditioning, and the number of linear iterations to allow.

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`.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

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). Although some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL), PCG should *only* be used with these packages when the linear systems are known to be *symmetric*. Since the scaling of matrix rows and columns must be identical in a symmetric matrix, symmetric preconditioning should work appropriately even for packages designed with one-sided preconditioning in mind.

```
SUNLinearSolver SUNPCG(N_Vector y, int pretype, int maxl);
```

- `SUNPCGSetPrecType`

This function updates the flag indicating use of preconditioning. As above, any one of the input values, `PREC_LEFT` (1), `PREC_RIGHT` (2), or `PREC_BOTH` (3) will enable preconditioning; `PREC_NONE` (0) disables preconditioning.

This routine will return with one of the error codes `SUNLS_ILL_INPUT` (illegal `pretype`), `SUNLS_MEM_NULL` (`S` is `NULL`), or `SUNLS_SUCCESS`.

```
int SUNPCGSetPrecType(SUNLinearSolver S, int pretype);
```

- `SUNPCGSetMaxl`

This function updates the number of linear solver iterations to allow.

A `maxl` argument that is  $\leq 0$  will result in the default value (5).

This routine will return with one of the error codes `SUNLS_MEM_NULL` (`S` is `NULL`) or `SUNLS_SUCCESS`.

```
int SUNPCGSetMaxl(SUNLinearSolver S, int maxl);
```

For solvers that include a Fortran interface module, the `SUNLINSOL_PCG` module also includes the Fortran-callable function `FSUNPCGInit(code, pretype, maxl, ier)` to initialize this `SUNLINSOL_PCG` 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`); `pretype` and `maxl` are the same as for the C function `SUNPCG`; `ier` is an error return flag equal to 0 for success and -1 for failure. All of these input arguments should be declared so as to match C type `int`. This routine must be called *after* the `NVECTOR` object has been initialized. Additionally, when using `ARKODE` with a non-identity mass matrix, the Fortran-callable function `FSUNMassPCGInit(pretype, maxl, ier)` initializes this `SUNLINSOL_PCG` module for solving mass matrix linear systems.

The `SUNPCGSetPrecType` and `SUNPCGSetMaxl` routines also support Fortran interfaces for the system and mass matrix solvers (all arguments should be commensurate with a C `int`):

- `FSUNPCGSetPrecType(code, pretype, ier)`
- `FSUNMassPCGSetPrecType(pretype, ier)`
- `FSUNPCGSetMaxl(code, maxl, ier)`
- `FSUNMassPCGSetMaxl(maxl, ier)`

## 8.14 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  $10 \cdot \text{tol}$ , 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.

## 8.15 SUNLinearSolver functions used by CVODE

In Table 8.5, we list the linear solver functions in the `SUNLINSOL` module used within the `CVODE` package. The table also shows, for each function, which of the code modules uses the function. In general, the main `CVODE` integrator considers three categories of linear solvers, *direct*, *iterative* and *custom*, with interfaces accessible in the `CVODE` header files `cvode/cvode_direct.h` (CVDLS), `cvode/cvode_spils.h` (CVSPILS) and `cvode/cvode_customls.h` (CVCLS), respectively. Hence, the table columns reference the use of `SUNLINSOL` functions by each of these solver interfaces.

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.

Table 8.5: List of linear solver functions usage by `CVODE` code modules

|                                         | CVDLS | CVSPILS | CVCLS |
|-----------------------------------------|-------|---------|-------|
| <code>SUNLinSolGetType</code>           | ✓     | ✓       | †     |
| <code>SUNLinSolSetATimes</code>         |       | ✓       | †     |
| <code>SUNLinSolSetPreconditioner</code> |       | ✓       | †     |
| <code>SUNLinSolSetScalingVectors</code> |       | ✓       | †     |
| <code>SUNLinSolInitialize</code>        | ✓     | ✓       | ✓     |
| <code>SUNLinSolSetup</code>             | ✓     | ✓       | ✓     |
| <code>SUNLinSolSolve</code>             | ✓     | ✓       | ✓     |
| <code>SUNLinSolNumIters</code>          |       | ✓       | †     |
| <code>SUNLinSolResNorm</code>           |       | ✓       | †     |
| <code>SUNLinSolResid</code>             |       | ✓       | †     |
| <code>SUNLinSolLastFlag</code>          |       |         |       |
| <code>SUNLinSolFree</code>              | ✓     | ✓       | ✓     |
| <code>SUNLinSolSpace</code>             |       | †       | †     |

The linear solver functions listed in Table 8.2 with a † symbol are optionally used, in that these are only called if they are implemented in the `SUNLINSOL` module that is being used (i.e. their function

pointers are non-NULL). Also, although CVODE does not call **SUNLinSolLastFlag** directly, this routine is available for users to query linear solver issues directly.

## Chapter 9

# Description of the SUNNonlinearSolver module

SUNDIALS time integration packages are written in terms of generic nonlinear solver operations defined by the SUNNONLINSOL API and implemented by a particular SUNNONLINSOL module of type `SUNNonlinearSolver`. Users can supply their own SUNNONLINSOL module, or use one of the modules provided with SUNDIALS.

The time integrators in SUNDIALS specify a default nonlinear solver module and as such this chapter is intended for users that wish to use a non-default nonlinear solver module or would like to provide their own nonlinear solver implementation. Users interested in using a non-default solver module may skip the description of the SUNNONLINSOL API in section 9.1 and proceed 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. Finally, section 9.1.7 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  $G(y) = y$ .

**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`.

**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`.

**SUNNonlinSolSolve**

Call            `retval = SUNNonlinSolSolve(NLS, y0, y, w, tol, callLSetup, mem);`

Description   The *required* function `SUNNonlinSolSolve` solves the nonlinear system  $F(y) = 0$  or  $G(y) = y$ .

Arguments    `NLS` (`SUNNonlinearSolver`) a `SUNNONLINSOL` object.

`y0` (`N_Vector`) the initial iterate for the nonlinear solve. This *must* remain unchanged throughout the solution process.

`y` (`N_Vector`) the solution to the nonlinear system.

`w` (`N_Vector`) the solution error weight vector used for computing weighted error norms.

`tol` (`realtype`) the requested solution tolerance in the weighted root-mean-squared norm.

`callLSetup` (`booleantype`) a flag indicating that the integrator recommends for the linear solver setup function to be called.

**mem** (void \*) the SUNDIALS integrator memory structure.

**Return value** The return value **retval** (of type **int**) is zero for a successful solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

#### SUNNonlinSolFree

**Call** **retval** = SUNNonlinSolFree(NLS);

**Description** The *optional* function **SUNNonlinSolFree** frees any memory allocated by the nonlinear solver.

**Arguments** **NLS** (**SUNNonlinearSolver**) a SUNNONLINSOL object.

**Return value** The return value **retval** (of type **int**) should be zero for a successful call, and a negative value for a failure. SUNNONLINSOL implementations that do not allocate data may set this operation to **NULL**.

### 9.1.2 SUNNonlinearSolver set functions

The following set functions are used to supply nonlinear solver modules with functions defined by the SUNDIALS integrators and to modify solver parameters. Only the routine for setting the nonlinear system defining function (**SUNNonlinSolSetSysFn**) is required. All other set functions are optional.

#### SUNNonlinSolSetSysFn

**Call** **retval** = SUNNonlinSolSetSysFn(NLS, SysFn);

**Description** The *required* function **SUNNonlinSolSetSysFn** is used to provide the nonlinear solver with the function defining the nonlinear system. This is the function  $F(y)$  in  $F(y) = 0$  for **SUNNONLINEARSOLVER\_ROOTFIND** modules or  $G(y)$  in  $G(y) = y$  for **SUNNONLINEARSOLVER\_FIXEDPOINT** modules.

**Arguments** **NLS** (**SUNNonlinearSolver**) a SUNNONLINSOL object.

**SysFn** (**SUNNonlinSolSysFn**) the function defining the nonlinear system. See section 9.1.4 for the definition of **SUNNonlinSolSysFn**.

**Return value** The return value **retval** (of type **int**) should be zero for a successful call, and a negative value for a failure.

#### SUNNonlinSolSetLSetupFn

**Call** **retval** = SUNNonlinSolSetLSetupFn(NLS, LSetupFn);

**Description** The *optional* function **SUNNonlinSolLSetupFn** is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver setup function.

**Arguments** **NLS** (**SUNNonlinearSolver**) a SUNNONLINSOL object.

**LSetupFn** (**SUNNonlinSolLSetupFn**) a wrapper function to the SUNDIALS integrator's linear solver setup function. See section 9.1.4 for the definition of **SUNNonlinLSetupFn**.

**Return value** The return value **retval** (of type **int**) should be zero for a successful call, and a negative value for a failure.

**Notes** The **SUNNonlinLSetupFn** function sets up the linear system  $Ax = b$  where  $A = \frac{\partial F}{\partial y}$  is the linearization of the nonlinear residual function  $F(y) = 0$  (when using **SUNLINSOL** direct linear solvers) or calls the user-defined preconditioner setup function (when using **SUNLINSOL** iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize **SUNLINSOL** linear solvers, or use **SUNLINSOL** linear solvers that do not require setup may set this operation to **NULL**.

**SUNNonlinSolSetLSolveFn**

|              |                                                                                                                                                                                                                                                                                                                                                                                  |
|--------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Call         | <code>retval = SUNNonlinSolSetLSolveFn(NLS, LSolveFn);</code>                                                                                                                                                                                                                                                                                                                    |
| Description  | The <i>optional</i> function <code>SUNNonlinSolSetLSolveFn</code> is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver solve function.                                                                                                                                                                                             |
| Arguments    | <code>NLS</code> ( <code>SUNNonlinearSolver</code> ) a <code>SUNNONLINSOL</code> object<br><code>LSolveFn</code> ( <code>SUNNonlinSolLSolveFn</code> ) a wrapper function to the SUNDIALS integrator's linear solver solve function. See section 9.1.4 for the definition of <code>SUNNonlinSolLSolveFn</code> .                                                                 |
| 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        | The <code>SUNNonlinLSolveFn</code> function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ . <code>SUNNONLINSOL</code> implementations that do not require solving this system or do not use <code>SUNLINSOL</code> linear solvers may set this operation to <code>NULL</code> . |

**SUNNonlinSolSetConvTestFn**

|              |                                                                                                                                                                                                                                                                                                                                |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Call         | <code>retval = SUNNonlinSolSetConvTestFn(NLS, CTestFn);</code>                                                                                                                                                                                                                                                                 |
| Description  | The <i>optional</i> function <code>SUNNonlinSolSetConvTestFn</code> 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    | <code>NLS</code> ( <code>SUNNonlinearSolver</code> ) a <code>SUNNONLINSOL</code> object.<br><code>CTestFn</code> ( <code>SUNNonlineSolConvTestFn</code> ) a SUNDIALS integrator's nonlinear solver convergence test function. See section 9.1.4 for the definition of <code>SUNNonlinSolConvTestFn</code> .                    |
| 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        | <code>SUNNONLINSOL</code> implementations utilizing their own convergence test criteria may set this function to <code>NULL</code> .                                                                                                                                                                                           |

**SUNNonlinSolSetMaxIters**

|              |                                                                                                                                                                                                                                                      |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Call         | <code>retval = SUNNonlinSolSetMaxIters(NLS, maxiters);</code>                                                                                                                                                                                        |
| Description  | The <i>optional</i> function <code>SUNNonlinSolSetMaxIters</code> 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    | <code>NLS</code> ( <code>SUNNonlinearSolver</code> ) a <code>SUNNONLINSOL</code> object.<br><code>maxiters</code> ( <code>int</code> ) the maximum number of nonlinear iterations.                                                                   |
| 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 (e.g., <code>maxiters &lt; 1</code> ).                                                                     |

### 9.1.3 SUNNonlinearSolver get functions

The following get functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routine for getting the current total number of iterations (`SUNNonlinSolGetNumIters` is optional. The routine for getting the current nonlinear solver iteration (`SUNNonlinSolGetCurIter`) is required when using the convergence test provided by the SUNDIALS integrator or when using a `SUNLINSOL` spils linear solver otherwise, `SUNNonlinSolGetCurIter` is optional.

**SUNNonlinSolGetNumIters**

|              |                                                                                                                                                                                                                                                              |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Call         | <code>retval = SUNNonlinSolGetNumIters(NLS, numiters);</code>                                                                                                                                                                                                |
| Description  | The <i>optional</i> function <code>SUNNonlinSolGetNumIters</code> 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    | <code>NLS</code> ( <code>SUNNonlinearSolver</code> ) a <code>SUNNONLINSOL</code> object<br><code>numiters</code> ( <code>long int*</code> ) the total number of nonlinear solver iterations.                                                                 |
| 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.                                                                                                                   |

**SUNNonlinSolGetCurIter**

|              |                                                                                                                                                                                                                                                                           |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Call         | <code>retval = SUNNonlinSolGetCurIter(NLS, iter);</code>                                                                                                                                                                                                                  |
| Description  | The function <code>SUNNonlinSolGetCurIter</code> returns the iteration index of the current nonlinear solve. This function is <i>required</i> when using SUNDIALS integrator-provided convergence tests and <i>optional</i> for user supplied convergence test functions. |
| Arguments    | <code>NLS</code> ( <code>SUNNonlinearSolver</code> ) a <code>SUNNONLINSOL</code> object<br><code>iter</code> ( <code>int*</code> ) the nonlinear solver iteration in the current solve starting from zero.                                                                |
| 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.                                                                                                                                |

**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   | <code>typedef int (*SUNNonlinSolSysFn)(N_Vector y, N_Vector F, void* mem);</code>                                                                                                                                                                                                                                          |
| Purpose      | These functions evaluate the nonlinear system $F(y)$ for <code>SUNNONLINEARSOLVER_ROOTFIND</code> type modules or $G(y)$ for <code>SUNNONLINEARSOLVER_FIXEDPOINT</code> type modules. Memory for <code>F</code> must be allocated prior to calling this function. The vector <code>y</code> <i>must</i> be left unchanged. |
| Arguments    | <code>y</code> is the state vector at which the nonlinear system should be evaluated.<br><code>F</code> is the output vector containing $F(y)$ or $G(y)$ , depending on the solver type.<br><code>mem</code> is the SUNDIALS integrator memory structure.                                                                  |
| Return value | The return value <code>retval</code> (of type <code>int</code> ) is zero for a successful solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.                                                                                                                                |

**SUNNonlinSolLSetupFn**

|            |                                                                                                                                                                                                                       |
|------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Definition | <code>typedef int (*SUNNonlinSolLSetupFn)(N_Vector y, N_Vector F,<br/>                                          booleantype jbad,<br/>                                          booleantype* jcur, void* mem);</code> |
| Purpose    | These functions are wrappers to the SUNDIALS integrator's function for setting up linear solves with <code>SUNLINSOL</code> modules.                                                                                  |

|              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Arguments    | <p><b>y</b> is the state vector at which the linear system should be setup.</p> <p><b>F</b> is the value of the nonlinear system function at <b>y</b>.</p> <p><b>jbad</b> is an input indicating whether the nonlinear solver believes that <math>A</math> has gone stale (SUNTRUE) or not (SUNFALSE).</p> <p><b>jcur</b> is an output indicating whether the routine has updated the Jacobian <math>A</math> (SUNTRUE) or not (SUNFALSE).</p> <p><b>mem</b> is the SUNDIALS integrator memory structure.</p>                                    |
| Return value | The return value <b>retval</b> (of type <b>int</b> ) is zero for a successful solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.                                                                                                                                                                                                                                                                                                                                                                  |
| Notes        | The <b>SUNNonlinLSetupFn</b> function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLINSOL direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLINSOL iterative linear solvers). SUNNONLINSOL implementations that do not require solving this system, do not utilize SUNLINSOL linear solvers, or use SUNLINSOL linear solvers that do not require setup may ignore these functions. |

#### SUNNonlinSolLSolveFn

|              |                                                                                                                                                                                                                                                                                                                                |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Definition   | <code>typedef int (*SUNNonlinSolLSolveFn)(N_Vector y, N_Vector b, void* mem);</code>                                                                                                                                                                                                                                           |
| Purpose      | These functions are wrappers to the SUNDIALS integrator's function for solving linear systems with SUNLINSOL modules.                                                                                                                                                                                                          |
| Arguments    | <p><b>y</b> is the input vector containing the current nonlinear iteration.</p> <p><b>b</b> contains the right-hand side vector for the linear solve on input and the solution to the linear system on output.</p> <p><b>mem</b> is the SUNDIALS integrator memory structure.</p>                                              |
| Return value | The return value <b>retval</b> (of type <b>int</b> ) is zero for a successful solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.                                                                                                                                                |
| Notes        | The <b>SUNNonlinLSolveFn</b> function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ . SUNNONLINSOL implementations that do not require solving this system or do not use SUNLINSOL linear solvers may ignore these functions. |

#### SUNNonlinSolConvTestFn

|              |                                                                                                                                                                                                                                                                                                                                                                                    |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Definition   | <code>typedef int (*SUNNonlinSolConvTestFn)(SUNNonlinearSolver NLS, N_Vector y, N_Vector del, realtype tol, N_Vector ewt, void* mem);</code>                                                                                                                                                                                                                                       |
| 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    | <p><b>NLS</b> is the SUNNONLINSOL object.</p> <p><b>y</b> is the current nonlinear iterate.</p> <p><b>del</b> is the difference between the current and prior nonlinear iterates.</p> <p><b>tol</b> is the nonlinear solver tolerance.</p> <p><b>ewt</b> is the weight vector used in computing weighted norms.</p> <p><b>mem</b> is the SUNDIALS integrator memory structure.</p> |
| Return value | The return value of this routine will be a negative value if an unrecoverable error occurred or one of the following:<br><b>SUN-NLS-SUCCESS</b> 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 <b>ewt</b> . 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   | 1     | the nonlinear solver is not converged, keep iterating        |
| SUN-NLS_CONV_RECVR | 2     | the nonlinear solver appears to be diverging, try to recover |
| SUN-NLS_MEM_NULL   | -1    | a memory argument is NULL                                    |
| SUN-NLS_MEM_FAIL   | -2    | a memory access or allocation failed                         |
| SUN-NLS_ILL_INPUT  | -3    | an illegal input option was provided                         |

### 9.1.6 The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNONLINSOL implementations through the generic 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 (*setlssetupfn)(SUNNonlinearSolver, SUNNonlinSolLSSetupFn);
    int (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
    int (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn);
    int (*setmaxiters)(SUNNonlinearSolver, int);
```

```

    int                (*getnumiters)(SUNNonlinearSolver, long int*);
    int                (*getcuriter)(SUNNonlinearSolver, int*);
};

```

The generic SUNNONLINSOL module defines and implements the nonlinear solver operations defined in Sections 9.1.1 – 9.1.3. These routines are in fact only wrappers to the nonlinear solver operations provided by a particular SUNNONLINSOL implementation, which are accessed through the ops field of the `SUNNonlinearSolver` structure. To illustrate this point we show below the implementation of a typical nonlinear solver operation from the generic SUNNONLINSOL module, namely `SUNNonlinSolSolve`, which solves the nonlinear system and returns a flag denoting a successful or failed solve:

```

int SUNNonlinSolSolve(SUNNonlinearSolver NLS,
                     N_Vector y0, N_Vector y,
                     N_Vector w, realtype tol,
                     booleantype callLSetup, void* mem)
{
    return((int) NLS->ops->solve(NLS, y0, y, w, tol, callLSetup, mem));
}

```

### 9.1.7 Implementing a Custom SUNNonlinearSolver Module

A SUNNONLINSOL implementation *must* do the following:

1. Specify the content of the SUNNONLINSOL module.
2. Define and implement the required nonlinear solver operations defined in Sections 9.1.1 – 9.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one SUNNONLINSOL module (each with different `SUNNonlinearSolver` internal data representations) in the same code.
3. Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

1. Define and implement additional user-callable “set” routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.
2. Provide additional user-callable “get” routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

## 9.2 The SUNNonlinearSolver\_Newton implementation

This section describes the SUNNONLINSOL implementation of Newton’s method. To access the 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.

### 9.2.1 SUNNonlinearSolver\_Newton description

To find the solution to

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

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

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

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

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

in which  $A$  is the Jacobian matrix

$$A \equiv \partial F / \partial y. \quad (9.4)$$

Depending on the linear solver used, the `SUNNONLINSOL_NEWTON` module will employ either a Modified Newton method, or an Inexact Newton method [4, 7, 15, 17, 30]. When used with a direct linear solver, the Jacobian matrix  $A$  is held constant during the Newton iteration, resulting in a Modified Newton method. With a matrix-free iterative linear solver, the iteration is an Inexact Newton method.

In both cases, calls to the integrator-supplied `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 `SUNNonlinSolSetConvTest` functions after attaching the `SUNNONLINSOL_NEWTON` object to the integrator.

### 9.2.2 SUNNonlinearSolver\_Newton functions

The `SUNNONLINSOL_NEWTON` module provides the following constructor for creating the `SUNNonlinearSolver` object.

|                                  |
|----------------------------------|
| <code>SUNNonlinSol_Newton</code> |
|----------------------------------|

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`.

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<br><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> . |

### 9.2.3 SUNNonlinearSolver\_Newton content

The *content* field of the `SUNNONLINSOL_NEWTON` module is 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;
};
```

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

|                       |                                                                                         |
|-----------------------|-----------------------------------------------------------------------------------------|
| <code>Sys</code>      | - the function for evaluating the nonlinear system,                                     |
| <code>LSetup</code>   | - the package-supplied function for setting up the linear solver,                       |
| <code>LSolve</code>   | - the package-supplied function for performing a linear solve,                          |
| <code>CTest</code>    | - the function for checking convergence of the Newton iteration,                        |
| <code>delta</code>    | - the Newton iteration update vector,                                                   |
| <code>jcur</code>     | - the Jacobian status ( <code>SUNTRUE</code> = current, <code>SUNFALSE</code> = stale), |
| <code>curiter</code>  | - the current number of iterations in the solve attempt,                                |
| <code>maxiters</code> | - the maximum number of Newton iterations allowed in a solve, and                       |
| <code>niters</code>   | - the total number of nonlinear iterations across all solves.                           |

### 9.2.4 SUNNonlinearSolver\_Newton Fortran interface

For SUNDIALS integrators that include a Fortran 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 FSUNNEWTONINIT 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 (int*)</code> is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).                                                                                             |
| 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 The SUNNonlinearSolver\_FixedPoint implementation

This section describes the SUNNONLINSOL implementation of a fixed point (functional) iteration with optional Anderson acceleration. To access the SUNNONLINSOL\_FIXEDPOINT module, include the header file `sunnonlinsol/sunnonlinsol.fixedpoint.h`. We note that the SUNNONLINSOL\_FIXEDPOINT module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolfixedpoint` module library.

#### 9.3.1 SUNNonlinearSolver\_FixedPoint description

To find the solution to

$$G(y) = y \quad (9.5)$$

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

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

where  $n$  is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [3, 38, 18, 32]. With Anderson acceleration using subspace size  $m$ , the series of approximate solutions can be formulated as the linear combination

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

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

$$\alpha^{(n)} = (\alpha_0^{(n)}, \dots, \alpha_{m_n}^{(n)}) \quad (9.8)$$

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

$$F_n = (f_{n-m_n}, \dots, f_n) \quad (9.9)$$

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

Following the recommendations made in [38], the SUNNONLINSOL\_FIXEDPOINT implementation computes the series of approximate solutions as

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

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

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

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

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

with  $\Delta f_i = f_{i+1} - f_i$ . The least-squares problem is solved by applying a QR factorization to  $\Delta F_n = Q_n R_n$  and solving  $R_n \gamma = Q_n^T f_n$ .

The acceleration subspace size  $m$  is required when constructing the `SUNNONLINSOL_FIXEDPOINT` object. The default maximum number of iterations and the stopping criteria for the fixed point iteration are supplied by the `SUNDIALS` integrator when `SUNNONLINSOL_FIXEDPOINT` is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling `SUNNonlinSolSetMaxIters` and `SUNNonlinSolSetConvTest` functions after attaching the `SUNNONLINSOL_FIXEDPOINT` object to the integrator.

### 9.3.2 SUNNonlinearSolver\_FixedPoint functions

The `SUNNONLINSOL_FIXEDPOINT` module provides the following constructor for creating the `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`.

Since the accelerated fixed point iteration (9.6) does not require the setup or solution of any linear systems, the `SUNNONLINSOL_FIXEDPOINT` module implements all of the functions defined in sections 9.1.1 – 9.1.3 except for the `SUNNonlinSolSetup`, `SUNNonlinSolSetLSetupFn`, and `SUNNonlinSolSetLSolveFn` functions, that are set to `NULL`. The `SUNNONLINSOL_FIXEDPOINT` functions have the same names as those defined by the generic `SUNNONLINSOL` API with `_FixedPoint` appended to the function name. Unless using the `SUNNONLINSOL_FIXEDPOINT` module as a standalone nonlinear solver the generic functions defined in sections 9.1.1 – 9.1.3 should be called in favor of the `SUNNONLINSOL_FIXEDPOINT`-specific implementations.

The `SUNNONLINSOL_FIXEDPOINT` module also defines the following additional user-callable function.

#### `SUNNonlinSolGetSysFn_FixedPoint`

- Call `retval = SUNNonlinSolGetSysFn_FixedPoint(NLS, SysFn);`
- Description The function `SUNNonlinSolGetSysFn_FixedPoint` returns the fixed-point function that defines the nonlinear system.
- Arguments `NLS` (`SUNNonlinearSolver`) a `SUNNONLINSOL` object  
`SysFn` (`SUNNonlinSolSysFn*`) the function defining the nonlinear system.
- Return value The return value `retval` (of type `int`) should be zero for a successful call, and a negative value for a failure.
- Notes This function is intended for users that wish to evaluate the fixed-point function in a custom convergence test function for the `SUNNONLINSOL_FIXEDPOINT` module. We note that `SUNNONLINSOL_FIXEDPOINT` will not leverage the results from any user calls to `SysFn`.

### 9.3.3 SUNNonlinearSolver\_FixedPoint content

The *content* field of the `SUNNONLINSOL_FIXEDPOINT` module is 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;
};

```

The following entries of the *content* field are always allocated:

**Sys** - function for evaluating the nonlinear system,  
**CTest** - function for checking convergence of the fixed point iteration,  
**yprev** - **N\_Vector** used to store previous fixed-point iterate,  
**gy** - **N\_Vector** used to store  $G(y)$  in fixed-point algorithm,  
**delta** - **N\_Vector** used to store difference between successive fixed-point iterates,  
**curiter** - the current number of iterations in the solve attempt,  
**maxiters** - the maximum number of fixed-point iterations allowed in a solve, and  
**niters** - the total number of nonlinear iterations across all solves.

**m** - number of acceleration vectors,

If Anderson acceleration is requested (i.e.,  $m > 0$  in the call to `SUNNonlinSol_FixedPoint`), then the following items are also allocated within the *content* field:

**imap** - index array used in acceleration algorithm (length **m**)  
**R** - small matrix used in acceleration algorithm (length **m\*m**)  
**gamma** - small vector used in acceleration algorithm (length **m**)  
**cvals** - small vector used in acceleration algorithm (length **m+1**)  
**df** - array of **N\_Vectors** used in acceleration algorithm (length **m**)  
**dg** - array of **N\_Vectors** used in acceleration algorithm (length **m**)  
**q** - array of **N\_Vectors** used in acceleration algorithm (length **m**)  
**Xvecs** - **N\_Vector** pointer array used in acceleration algorithm (length **m+1**)  
**fold** - **N\_Vector** used in acceleration algorithm  
**gold** - **N\_Vector** used in acceleration algorithm

### 9.3.4 SUNNonlinearSolver\_FixedPoint Fortran interface

For SUNDIALS integrators that include a Fortran interface, the SUNNONLINSOL\_FIXEDPOINT module also includes a Fortran-callable function for creating a `SUNNonlinearSolver` object.

|                           |
|---------------------------|
| <b>FSUNFIXEDPOINTINIT</b> |
|---------------------------|

Call `FSUNFIXEDPOINTINIT(code, m, ier);`

Description The function `FSUNFIXEDPOINTINIT` can be called for Fortran programs to create a `SUNNonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form  $G(y) = y$ .

Arguments `code` (`int*`) is an integer input specifying the solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, and 4 for ARKODE).

`m` (`int*`) is an integer input specifying the number of acceleration vectors.

Return value `ier` is a return completion flag equal to 0 for a success return and -1 otherwise. See printed message for details in case of failure.



## 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/lib`, with *instdir* 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 3.0.2 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. While many Linux distributions offer CMake, the version included may be out of date. CMake is continually adding new features, and the latest version can be downloaded from <http://www.cmake.org>. Build instructions for CMake (only necessary for Unix-like systems) can be found on the CMake website. Once CMake is installed, Linux/Unix users will be able to use **ccmake**, while Windows users will be able to use **CMakeSetup**.

As previously noted, when using CMake to configure, build and install SUNDIALS, it is always required to use a separate build directory. While in-source builds are possible, they are explicitly prohibited by the SUNDIALS CMake scripts (one of the reasons being that, unlike autotools, CMake does not provide a **make distclean** procedure and it is therefore difficult to clean-up the source tree after an in-source build). By ensuring a separate build directory, it is an easy task for the user to clean-up all traces of the build by simply removing the build directory. CMake does generate a **make clean** which will remove files generated by the compiler and linker.

### A.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The *instdir* defaults to `/usr/local` and can be changed by setting the `CMAKE_INSTALL_PREFIX` variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the **cmake** command, or from a **curses**-based GUI by using the **ccmake** command. Examples for using both methods will be presented. For the examples shown it is assumed that there is a top level SUNDIALS directory with appropriate source, build and install directories:

```
% mkdir (...)sundials/instdir
% mkdir (...)sundials/builddir
% cd (...)sundials/builddir
```

#### Building with the GUI

Using CMake with the GUI follows this general process:

- Select and modify values, run configure (c key)
- New values are denoted with an asterisk
- To set a variable, move the cursor to the variable and press enter
  - If it is a boolean (ON/OFF) it will toggle the value
  - If it is string or file, it will allow editing of the string

- For file and directories, the <tab> key can be used to complete
- Repeat until all values are set as desired and the generate option is available (g key)
- Some variables (advanced variables) are not visible right away
- To see advanced variables, toggle to advanced mode (t key)
- To search for a variable press / key, and to repeat the search, press the n key

To build the default configuration using the GUI, from the *builddir* enter the *ccmake* command and point to the *solverdir*:

```
% ccmake ../solverdir
```

The default configuration screen is shown in Figure A.1.

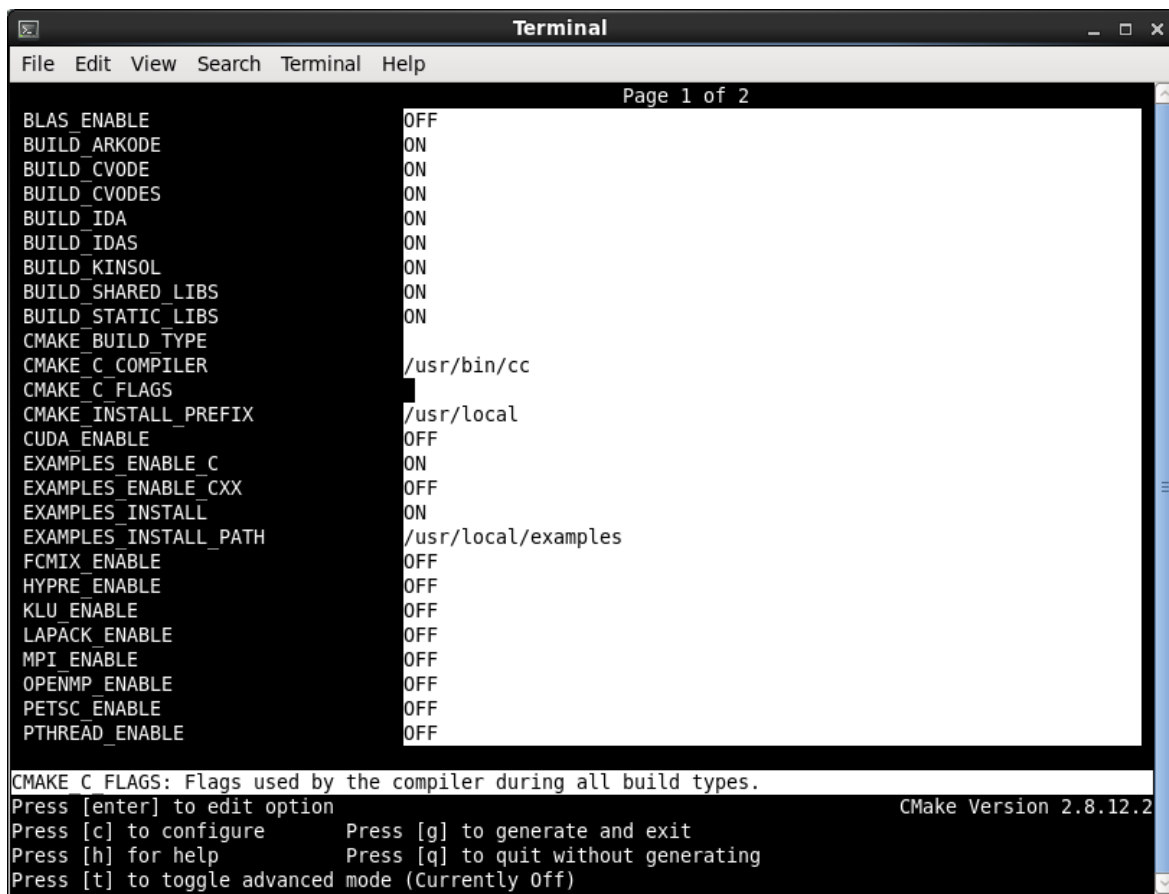


Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instdir* for both SUNDIALS and corresponding examples can be changed by setting the *CMAKE\_INSTALL\_PREFIX* and the *EXAMPLES\_INSTALL\_PATH* as shown in figure A.2.

Pressing the (g key) will generate makefiles including all dependencies and all rules to build SUNDIALS on this system. Back at the command prompt, you can now run:

```
% make
```

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

```
% make install
```

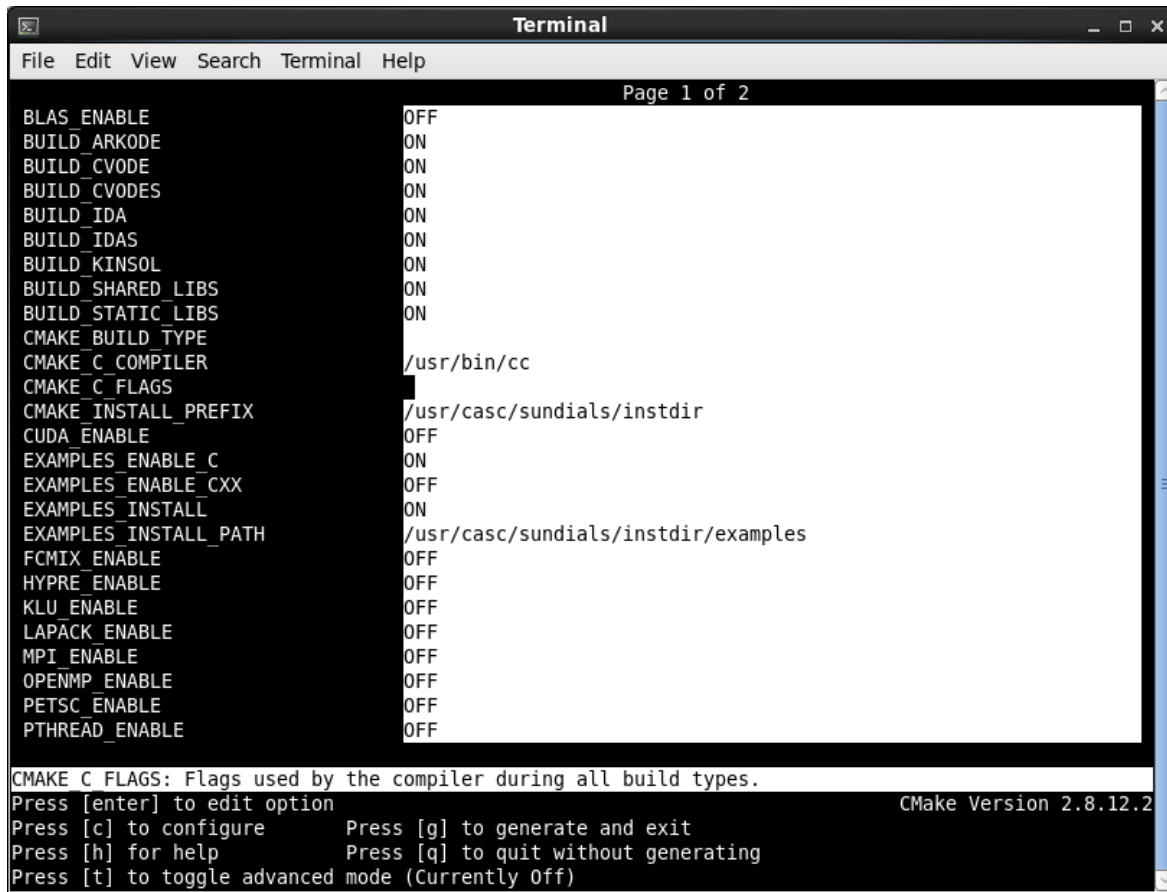


Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

### Building from the command line

Using CMake from the command line is simply a matter of specifying CMake variable settings with the `cmake` command. The following will build the default configuration:

```

% cmake -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> ../solverdir
% make
% make install

```

### A.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

**BLAS\_ENABLE** - Enable BLAS support

Default: OFF

Note: Setting this option to ON will trigger additional CMake options. See additional information on building with BLAS enabled in [A.1.4](#).

**BLAS\_LIBRARIES** - BLAS library

Default: /usr/lib/libblas.so

Note: CMake will search for libraries in your `LD_LIBRARY_PATH` prior to searching default system paths.

`BUILD_ARKODE` - Build the ARKODE library  
Default: ON

`BUILD_CVODE` - Build the CVODE library  
Default: ON

`BUILD_CVODES` - Build the CVODES library  
Default: ON

`BUILD_IDA` - Build the IDA library  
Default: ON

`BUILD_IDAS` - Build the IDAS library  
Default: ON

`BUILD_KINSOL` - Build the KINSOL library  
Default: ON

`BUILD_SHARED_LIBS` - Build shared libraries  
Default: ON

`BUILD_STATIC_LIBS` - Build static libraries  
Default: ON

`CMAKE_BUILD_TYPE` - Choose the type of build, options are: `None` (`CMAKE_C_FLAGS` used), `Debug`, `Release`, `RelWithDebInfo`, and `MinSizeRel`  
Default:  
Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by `CMAKE_<language>_FLAGS`.

`CMAKE_C_COMPILER` - C compiler  
Default: `/usr/bin/cc`

`CMAKE_C_FLAGS` - Flags for C compiler  
Default:

`CMAKE_C_FLAGS_DEBUG` - Flags used by the C compiler during debug builds  
Default: `-g`

`CMAKE_C_FLAGS_MINSIZEREL` - Flags used by the C compiler during release minsize builds  
Default: `-Os -DNDEBUG`

`CMAKE_C_FLAGS_RELEASE` - Flags used by the C compiler during release builds  
Default: `-O3 -DNDEBUG`

`CMAKE_CXX_COMPILER` - C++ compiler  
Default: `/usr/bin/c++`  
Note: A C++ compiler (and all related options) are only triggered if C++ examples are enabled (`EXAMPLES_ENABLE_CXX` is ON). All SUNDIALS solvers can be used from C++ applications by default without setting any additional configuration options.

`CMAKE_CXX_FLAGS` - Flags for C++ compiler  
Default:

`CMAKE_CXX_FLAGS_DEBUG` - Flags used by the C++ compiler during debug builds  
Default: `-g`

**CMAKE\_CXX\_FLAGS\_MINSIZEREL** - Flags used by the C++ compiler during release minsize builds

Default: -Os -DNDEBUG

**CMAKE\_CXX\_FLAGS\_RELEASE** - Flags used by the C++ compiler during release builds

Default: -O3 -DNDEBUG

**CMAKE\_Fortran\_COMPILER** - Fortran compiler

Default: /usr/bin/gfortran

Note: Fortran support (and all related options) are triggered only if either Fortran-C support is enabled (**FCMIX\_ENABLE** is ON) or BLAS/LAPACK support is enabled (**BLAS\_ENABLE** or **LAPACK\_ENABLE** is ON).

**CMAKE\_Fortran\_FLAGS** - Flags for Fortran compiler

Default:

**CMAKE\_Fortran\_FLAGS\_DEBUG** - Flags used by the Fortran compiler during debug builds

Default: -g

**CMAKE\_Fortran\_FLAGS\_MINSIZEREL** - Flags used by the Fortran compiler during release minsize builds

Default: -Os

**CMAKE\_Fortran\_FLAGS\_RELEASE** - Flags used by the Fortran compiler during release builds

Default: -O3

**CMAKE\_INSTALL\_PREFIX** - Install path prefix, prepended onto install directories

Default: /usr/local

Note: The user must have write access to the location specified through this option. Exported SUNDIALS header files and libraries will be installed under subdirectories **include** and **lib** of **CMAKE\_INSTALL\_PREFIX**, respectively.

**CUDA\_ENABLE** - Build the SUNDIALS CUDA vector module.

Default: OFF

**EXAMPLES\_ENABLE\_C** - Build the SUNDIALS C examples

Default: ON

**EXAMPLES\_ENABLE\_CUDA** - Build the SUNDIALS CUDA examples

Default: OFF

Note: You need to enable CUDA support to build these examples.

**EXAMPLES\_ENABLE\_CXX** - Build the SUNDIALS C++ examples

Default: OFF

**EXAMPLES\_ENABLE\_RAJA** - Build the SUNDIALS RAJA examples

Default: OFF

Note: You need to enable CUDA and RAJA support to build these examples.

**EXAMPLES\_ENABLE\_F77** - Build the SUNDIALS Fortran77 examples

Default: ON (if **FCMIX\_ENABLE** is ON)

**EXAMPLES\_ENABLE\_F90** - Build the SUNDIALS Fortran90 examples

Default: OFF

**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`.

`FCMIX_ENABLE` - Enable Fortran-C support

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 (build the parallel nvector).

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`), Fortran-C support is enabled (`FCMIX_ENABLE` is `ON`), and Fortran77 or Fortran90 examples are enabled (`EXAMPLES_ENABLE_F77` or `EXAMPLES_ENABLE_F90` are `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

`PETSC_ENABLE` - Enable PETSc support

Default: OFF

Note: See additional information on building with PETSc enabled in [A.1.4](#).

`PETSC_INCLUDE_DIR` - Path to PETSc header files

`PETSC_LIBRARY_DIR` - Path to PETSc installed library files

`PTHREAD_ENABLE` - Enable Pthreads support (build the Pthreads nvector).

Default: OFF

`RAJA_ENABLE` - Enable RAJA support (build the RAJA nvector).

Default: OFF

Note: You need to enable CUDA in order to build the RAJA vector module.

`SUNDIALS_F77_FUNC_CASE` - **advanced option** - Specify the case to use in the Fortran name-mangling scheme, options are: **lower** or **upper**

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (**lower**) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_UNDERSCORES` must also be set.

`SUNDIALS_F77_FUNC_UNDERSCORES` - **advanced option** - Specify the number of underscores to append in the Fortran name-mangling scheme, options are: **none**, **one**, or **two**

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (**one**) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_CASE` must also be set.

`SUNDIALS_INDEX_TYPE` - Integer type used for SUNDIALS indices, options are: `int32_t` or `int64_t`

Default: `int64_t`

`SUNDIALS_PRECISION` - Precision used in SUNDIALS, options are: **double**, **single**, or **extended**

Default: **double**

`SUPERLUMT_ENABLE` - Enable SuperLU\_MT support

Default: OFF

Note: See additional information on building with SuperLU\_MT enabled in [A.1.4](#).

`SUPERLUMT_INCLUDE_DIR` - Path to SuperLU\_MT header files (typically SRC directory)

`SUPERLUMT_LIBRARY_DIR` - Path to SuperLU\_MT installed library files

`SUPERLUMT_THREAD_TYPE` - Must be set to Pthread or OpenMP

Default: Pthread

`USE_GENERIC_MATH` - Use generic (stdc) math libraries

Default: ON



### xSDK Configuration Options

SUNDIALS supports CMake configuration options defined by the Extreme-scale Scientific Software Development Kit (xSDK) community policies (see <https://xsdk.info> for more information). xSDK CMake options are unused by default but may be activated by setting `USE_XSDK_DEFAULTS` to ON.

When xSDK options are active, they will overwrite the corresponding SUNDIALS option and may have different default values (see details below). As such the equivalent SUNDIALS options should not be used when configuring with xSDK options. In the GUI front end to CMake (`ccmake`), setting `USE_XSDK_DEFAULTS` to ON will hide the corresponding SUNDIALS options as advanced CMake variables. During configuration, messages are output detailing which xSDK flags are active and the equivalent SUNDIALS options that are replaced. Below is a complete list xSDK options and the corresponding SUNDIALS options if applicable.



**TPL\_BLAS\_LIBRARIES** - BLAS library

Default: `/usr/lib/libblas.so`

SUNDIALS equivalent: `BLAS_LIBRARIES`

Note: CMake will search for libraries in your `LD_LIBRARY_PATH` prior to searching default system paths.

**TPL\_ENABLE\_BLAS** - Enable BLAS support

Default: `OFF`

SUNDIALS equivalent: `BLAS_ENABLE`

**TPL\_ENABLE\_HYPRE** - Enable *hypre* support

Default: `OFF`

SUNDIALS equivalent: `HYPRE_ENABLE`

**TPL\_ENABLE\_KLU** - Enable KLU support

Default: `OFF`

SUNDIALS equivalent: `KLU_ENABLE`

**TPL\_ENABLE\_PETSC** - Enable PETSc support

Default: `OFF`

SUNDIALS equivalent: `PETSC_ENABLE`

**TPL\_ENABLE\_LAPACK** - Enable LAPACK support

Default: `OFF`

SUNDIALS equivalent: `LAPACK_ENABLE`

**TPL\_ENABLE\_SUPERLUMT** - Enable SuperLU-MT support

Default: `OFF`

SUNDIALS equivalent: `SUPERLUMT_ENABLE`

**TPL\_HYPRE\_INCLUDE\_DIRS** - Path to *hypre* header files

SUNDIALS equivalent: `HYPRE_INCLUDE_DIR`

**TPL\_HYPRE\_LIBRARIES** - *hypre* library

SUNDIALS equivalent: `N/A`

**TPL\_KLU\_INCLUDE\_DIRS** - Path to KLU header files

SUNDIALS equivalent: `KLU_INCLUDE_DIR`

**TPL\_KLU\_LIBRARIES** - KLU library

SUNDIALS equivalent: `N/A`

**TPL\_LAPACK\_LIBRARIES** - LAPACK (and BLAS) libraries

Default: `/usr/lib/liblapack.so;/usr/lib/libblas.so`

SUNDIALS equivalent: `LAPACK_LIBRARIES`

Note: CMake will search for libraries in your `LD_LIBRARY_PATH` prior to searching default system paths.

TPL\_PETSC\_INCLUDE\_DIRS - Path to PETSc header files  
SUNDIALS equivalent: PETSC\_INCLUDE\_DIR

TPL\_PETSC\_LIBRARIES - PETSc library  
SUNDIALS equivalent: N/A

TPL\_SUPERLUMT\_INCLUDE\_DIRS - Path to SuperLU\_MT header files  
SUNDIALS equivalent: SUPERLUMT\_INCLUDE\_DIR

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 interface  
Default: OFF  
SUNDIALS equivalent: FCMIX\_ENABLE

XSDK\_INDEX\_SIZE - Integer size (bits) used for indices in SUNDIALS, options are: 32 or 64  
Default: 32  
SUNDIALS equivalent: SUNDIALS\_INDEX\_TYPE

XSDK\_PRECISION - Precision used in SUNDIALS, options are: double, single, or quad  
Default: double  
SUNDIALS equivalent: SUNDIALS\_PRECISION

### A.1.3 Configuration examples

The following examples will help demonstrate usage of the CMake configure options. To configure SUNDIALS using the default C and Fortran compilers, and default mpicc and mpif77 parallel compilers, enable compilation of examples, and install libraries, headers, and example sources under subdirectories of /home/myname/sundials/, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> /home/myname/sundials/solverdir
%
% make install
%
```

To disable installation of the examples, use:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DMPI_ENABLE=ON \
> -DFCMIX_ENABLE=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/solverdir
```

```
%
% make install
%
```

### A.1.4 Working with external Libraries

The SUNDIALS suite contains many options to enable implementation flexibility when developing solutions. The following are some notes addressing specific configurations when using the supported third party libraries. When building SUNDIALS as a shared library external libraries any used with SUNDIALS must also be build as a shared library or as a static library compiled with the `-fPIC` flag.



#### Building with BLAS

SUNDIALS does not utilize BLAS directly but it may be needed by other external libraries that SUNDIALS can be built with (e.g. LAPACK, PETSc, SuperLU\_MT, etc.). To enable BLAS, set the `BLAS_ENABLE` option to `ON`. If the directory containing the BLAS library is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `BLAS_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the BLAS library in standard system locations. To explicitly tell CMake what libraries to use, the `BLAS_LIBRARIES` variable can be set to the desired library. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/myblaspath/lib/libblas.so \
> -DSUPERLUMT_ENABLE=ON \
> -DSUPERLUMT_INCLUDE_DIR=/mysuperlumtpath/SRC
> -DSUPERLUMT_LIBRARY_DIR=/mysuperlumtpath/lib
> /home/myname/sundials/solverdir
%
% make install
%
```

When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.



If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options `SUNDIALS_F77_FUNC.CASE` and `SUNDIALS_F77_FUNC.UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

#### Building with LAPACK

To enable LAPACK, set the `LAPACK_ENABLE` option to `ON`. If the directory containing the LAPACK library is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `LAPACK_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the `LAPACK_LIBRARIES` variable can be set to the desired libraries. When setting the LAPACK location explicitly the location of the corresponding BLAS library will also need to be set. Example:



```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DBLAS_ENABLE=ON \
> -DBLAS_LIBRARIES=/mylapackpath/lib/libblas.so \
> -DLAPACK_ENABLE=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/liblapack.so \
```

```
> /home/myname/sundials/solverdir
%
% make install
%
```



When allowing CMake to automatically locate the LAPACK library, CMake *may* also locate the corresponding BLAS library.

If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options `SUNDIALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one` respectively.

### Building with KLU

The KLU libraries are part of SuiteSparse, a suite of sparse matrix software, available from the Texas A&M University website: <http://faculty.cse.tamu.edu/davis/suitesparse.html>. SUNDIALS has been tested with SuiteSparse version 4.5.3. 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](http://crd-legacy.lbl.gov/~xiaoye/SuperLU/#superlu_mt). SUNDIALS has been tested with SuperLU\_MT version 3.1. To enable SuperLU\_MT, set `SUPERLUMT_ENABLE` to `ON`, set `SUPERLUMT_INCLUDE_DIR` to the `SRC` path of the SuperLU\_MT installation, and set the variable `SUPERLUMT_LIBRARY_DIR` to the `lib` path of the SuperLU\_MT installation. At the same time, the variable `SUPERLUMT_THREAD_TYPE` must be set to either `Pthread` or `OpenMP`.



Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either `OPENMP_ENABLE` or `PTHREAD_ENABLE` set to `ON` then SuperLU\_MT should be set to use the same threading type.

### Building with PETSc

The PETSc libraries are available for download from the Argonne National Laboratory website: <http://www.mcs.anl.gov/petsc>. SUNDIALS has been tested with PETSc version 3.7.2. To enable PETSc, set `PETSC_ENABLE` to `ON`, set `PETSC_INCLUDE_DIR` to the `include` path of the PETSc installation, and set the variable `PETSC_LIBRARY_DIR` to the `lib` path of the PETSc installation.

### Building with hypre

The *hypre* libraries are available for download from the Lawrence Livermore National Laboratory website: <http://computation.llnl.gov/projects/hypre>. SUNDIALS has been tested with *hypre* version 2.11.1. To enable *hypre*, set `HYPRE_ENABLE` to `ON`, set `HYPRE_INCLUDE_DIR` to the `include` path of the *hypre* installation, and set the variable `HYPRE_LIBRARY_DIR` to the `lib` path of the *hypre* installation.

### Building with CUDA

SUNDIALS CUDA modules and examples have been tested with version 8.0 of the CUDA toolkit. To build them, you need to install the Toolkit and compatible NVIDIA drivers. Both are available for download from the NVIDIA website: <https://developer.nvidia.com/cuda-downloads>. To enable CUDA, set `CUDA_ENABLE` to `ON`. If CUDA is installed in a nonstandard location, you may be prompted to

set the variable `CUDA_TOOLKIT_ROOT_DIR` with your CUDA Toolkit installation path. To enable CUDA examples, set `EXAMPLES_ENABLE_CUDA` to `ON`.

### Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from <https://github.com/LLNL/RAJA>. SUNDIALS RAJA modules and examples have been tested with RAJA version 0.3. 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_RAJA` to `ON`.

#### 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/lib* and *instdir/include*, respectively. The location can be changed by setting the CMake variable CMAKE\_INSTALL\_PREFIX. Although all installed libraries reside under *libdir/lib*, 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<br>sundials/sundials.fconfig.h<br>sundials/sundials.types.h<br>sundials/sundials.math.h<br>sundials/sundials.nvector.h<br>sundials/sundials.fnvector.h<br>sundials/sundials.matrix.h<br>sundials/sundials.linearsolver.h<br>sundials/sundials.iterative.h<br>sundials/sundials.direct.h<br>sundials/sundials.dense.h |
| <i>continued on next page</i> |              |                                                                                                                                                                                                                                                                                                                                                 |

|                                 |              |                                                                                                                            |
|---------------------------------|--------------|----------------------------------------------------------------------------------------------------------------------------|
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|                                 |              | sundials/sundials_band.h<br>sundials/sundials_nonlinearsolver.h<br>sundials/sundials_version.h                             |
| NVECTOR_SERIAL                  | Libraries    | libsundials_nvecserial. <i>lib</i> libsundials_fnvecserial.a                                                               |
|                                 | Header files | nvector/nvector_serial.h                                                                                                   |
| NVECTOR_PARALLEL                | Libraries    | libsundials_nvecparallel. <i>lib</i> libsundials_fnvecparallel.a                                                           |
|                                 | Header files | nvector/nvector_parallel.h                                                                                                 |
| NVECTOR_OPENMP                  | Libraries    | libsundials_nvecopenmp. <i>lib</i> libsundials_fnvecopenmp.a                                                               |
|                                 | Header files | nvector/nvector_openmp.h                                                                                                   |
| NVECTOR_PTHREADS                | Libraries    | libsundials_nvecpthreads. <i>lib</i> libsundials_fnvecpthreads.a                                                           |
|                                 | Header files | nvector/nvector_pthreads.h                                                                                                 |
| NVECTOR_PARHYP                  | Libraries    | libsundials_nvecparhyp. <i>lib</i>                                                                                         |
|                                 | Header files | nvector/nvector_parhyp.h                                                                                                   |
| NVECTOR_PETSC                   | Libraries    | libsundials_nvecpetsc. <i>lib</i>                                                                                          |
|                                 | Header files | nvector/nvector_petsc.h                                                                                                    |
| NVECTOR_CUDA                    | Libraries    | libsundials_nveccuda. <i>lib</i>                                                                                           |
|                                 | Header files | nvector/nvector_cuda.h<br>nvector/cuda/ThreadPartitioning.hpp<br>nvector/cuda/Vector.hpp<br>nvector/cuda/VectorKernels.cuh |
| NVECTOR_RAJA                    | Libraries    | libsundials_nvecraja. <i>lib</i>                                                                                           |
|                                 | Header files | nvector/nvector_raja.h<br>nvector/raja/Vector.hpp                                                                          |
| SUNMATRIX_BAND                  | Libraries    | libsundials_sunmatrixband. <i>lib</i><br>libsundials_fsunmatrixband.a                                                      |
|                                 | Header files | sunmatrix/sunmatrix_band.h                                                                                                 |
| SUNMATRIX_DENSE                 | Libraries    | libsundials_sunmatrixdense. <i>lib</i><br>libsundials_fsunmatrixdense.a                                                    |
|                                 | Header files | sunmatrix/sunmatrix_dense.h                                                                                                |
| SUNMATRIX_SPARSE                | Libraries    | libsundials_sunmatrixsparse. <i>lib</i><br>libsundials_fsunmatrixsparse.a                                                  |
|                                 | Header files | sunmatrix/sunmatrix_sparse.h                                                                                               |
| SUNLINSOL_BAND                  | Libraries    | libsundials_sunlinsolband. <i>lib</i><br>libsundials_fsunlinsolband.a                                                      |
|                                 | Header files | sunlinsol/sunlinsol_band.h                                                                                                 |
| SUNLINSOL_DENSE                 | Libraries    | libsundials_sunlinsoldense. <i>lib</i><br>libsundials_fsunlinsoldense.a                                                    |
|                                 | Header files | sunlinsol/sunlinsol_dense.h                                                                                                |
| SUNLINSOL_KLU                   | Libraries    | libsundials_sunlinsolklu. <i>lib</i><br>libsundials_fsunlinsolklu.a                                                        |
|                                 | Header files | sunlinsol/sunlinsol_klu.h                                                                                                  |
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| SUNLINSOL_LAPACKBAND            | Libraries    | libsundials_sunlinsollapackband. <i>lib</i><br>libsundials_fsunlinsollapackband.a       |                        |
|                                 | Header files | sunlinsol/sunlinsol_lapackband.h                                                        |                        |
| SUNLINSOL_LAPACKDENSE           | Libraries    | libsundials_sunlinsollapackdense. <i>lib</i><br>libsundials_fsunlinsollapackdense.a     |                        |
|                                 | Header files | sunlinsol/sunlinsol_lapackdense.h                                                       |                        |
| SUNLINSOL_PCG                   | Libraries    | libsundials_sunlinsolpcg. <i>lib</i><br>libsundials_fsunlinsolpcg.a                     |                        |
|                                 | Header files | sunlinsol/sunlinsol_pcg.h                                                               |                        |
| SUNLINSOL_SPBCGS                | Libraries    | libsundials_sunlinsolspbcgs. <i>lib</i><br>libsundials_fsunlinsolspbcgs.a               |                        |
|                                 | Header files | sunlinsol/sunlinsol_spbcgs.h                                                            |                        |
| SUNLINSOL_SPGMR                 | Libraries    | libsundials_sunlinsolspgmr. <i>lib</i><br>libsundials_fsunlinsolspgmr.a                 |                        |
|                                 | Header files | sunlinsol/sunlinsol_spgmr.h                                                             |                        |
| SUNLINSOL_SPGMR                 | Libraries    | libsundials_sunlinsolspgmr. <i>lib</i><br>libsundials_fsunlinsolspgmr.a                 |                        |
|                                 | Header files | sunlinsol/sunlinsol_spgmr.h                                                             |                        |
| SUNLINSOL_SPTFQMR               | Libraries    | libsundials_sunlinsolsptfqmr. <i>lib</i><br>libsundials_fsunlinsolsptfqmr.a             |                        |
|                                 | Header files | sunlinsol/sunlinsol_sptfqmr.h                                                           |                        |
| SUNLINSOL_SUPERLUMT             | Libraries    | libsundials_sunlinsolsuperlumt. <i>lib</i><br>libsundials_fsunlinsolsuperlumt.a         |                        |
|                                 | Header files | sunlinsol/sunlinsol_superlumt.h                                                         |                        |
| SUNNONLINSOL_NEWTON             | Libraries    | libsundials_sunnonlinsolnewton. <i>lib</i><br>libsundials_fsunnonlinsolnewton.a         |                        |
|                                 | Header files | sunnonlinsol/sunnonlinsol_newton.h                                                      |                        |
| SUNNONLINSOL_FIXEDPOINT         | Libraries    | libsundials_sunnonlinsolfixedpoint. <i>lib</i><br>libsundials_fsunnonlinsolfixedpoint.a |                        |
|                                 | Header files | sunnonlinsol/sunnonlinsol_fixedpoint.h                                                  |                        |
| CVODE                           | Libraries    | libsundials_cvode. <i>lib</i>                                                           | libsundials_fcvcde.a   |
|                                 | Header files | cvode/cvode.h                                                                           | cvode/cvode_impl.h     |
|                                 |              | cvode/cvode_direct.h                                                                    | cvode/cvode_spils.h    |
|                                 |              | cvode/cvode_bandpre.h                                                                   | cvode/cvode_bbdpre.h   |
| CVODES                          | Libraries    | libsundials_cvodes. <i>lib</i>                                                          |                        |
|                                 | Header files | cvodes/cvodes.h                                                                         | cvodes/cvodes_impl.h   |
|                                 |              | cvodes/cvodes_direct.h                                                                  | cvodes/cvodes_spils.h  |
|                                 |              | cvodes/cvodes_bandpre.h                                                                 | cvodes/cvodes_bbdpre.h |
| ARKODE                          | Libraries    | libsundials_arkode. <i>lib</i>                                                          | libsundials_farkode.a  |
|                                 | Header files | arkode/arkode.h                                                                         | arkode/arkode_impl.h   |
|                                 |              | arkode/arkode_direct.h                                                                  | arkode/arkode_spils.h  |
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|                                 |              | arkode/arkode.bandpre.h                          | arkode/arkode.bbdpre.h |
| IDA                             | Libraries    | libsundials_ida.lib                              | libsundials_fida.a     |
|                                 | Header files | ida/ida.h                                        | ida/ida_impl.h         |
|                                 |              | ida/ida_direct.h<br>ida/ida_bbdpre.h             | ida/ida_spils.h        |
| IDAS                            | Libraries    | libsundials_idas.lib                             |                        |
|                                 | Header files | idas/idas.h                                      | idas/idas_impl.h       |
|                                 |              | idas/idas_direct.h<br>idas/idas_bbdpre.h         | idas/idas_spils.h      |
| KINSOL                          | Libraries    | libsundials_kinsol.lib                           | libsundials_fkinsol.a  |
|                                 | Header files | kinsol/kinsol.h                                  | kinsol/kinsol_impl.h   |
|                                 |              | kinsol/kinsol_direct.h<br>kinsol/kinsol_bbdpre.h | kinsol/kinsol_spils.h  |



# 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 module |   |                                                 |
| 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_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.                                                         |

---

**CVDSL linear solver modules**


---

|                      |    |                                                                     |
|----------------------|----|---------------------------------------------------------------------|
| CVDSL_SUCCESS        | 0  | Successful function return.                                         |
| CVDSL_MEM_NULL       | -1 | The <code>cvode_mem</code> argument was NULL.                       |
| CVDSL_LMEM_NULL      | -2 | The CVDSL linear solver has not been initialized.                   |
| CVDSL_ILL_INPUT      | -3 | The CVDSL solver is not compatible with the current NVECTOR module. |
| CVDSL_MEM_FAIL       | -4 | A memory allocation request failed.                                 |
| CVDSL_JACFUNC_UNRECV | -5 | The Jacobian function failed in an unrecoverable manner.            |
| CVDSL_JACFUNC_RECVR  | -6 | The Jacobian function had a recoverable error.                      |
| CVDSL_SUNMAT_FAIL    | -7 | An error occurred with the current SUNMATRIX 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.           |

---



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**CVSPILS linear solver modules**

---

|                    |    |                                                                                                      |
|--------------------|----|------------------------------------------------------------------------------------------------------|
| CVSPILS_SUCCESS    | 0  | Successful function return.                                                                          |
| CVSPILS_MEM_NULL   | -1 | The <code>cvode_mem</code> argument was NULL.                                                        |
| CVSPILS_LMEM_NULL  | -2 | The CVSPILS linear solver has not been initialized.                                                  |
| CVSPILS_ILL_INPUT  | -3 | The CVSPILS solver is not compatible with the current NVECTOR module, or an input value was illegal. |
| CVSPILS_MEM_FAIL   | -4 | A memory allocation request failed.                                                                  |
| CVSPILS_PMEM_NULL  | -5 | The preconditioner module has not been initialized.                                                  |
| CVSPILS_SUNLS_FAIL | -6 | An error occurred with the current SUNLINSOL module.                                                 |



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