

# User Documentation for CVODES v3.1.0 (SUNDIALS v3.1.0)

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# Chapter 1

## Introduction

CVODES [34] is part of a software family called SUNDIALS: SUite of Nonlinear and Differential/ALgebraic equation Solvers [20]. This suite consists of CVODE, ARKODE, KINSOL and IDA, and variants of these with sensitivity analysis capabilities. CVODES is a solver for stiff and nonstiff initial value problems (IVPs) for systems of ordinary differential equation (ODEs). In addition to solving stiff and nonstiff ODE systems, CVODES has sensitivity analysis capabilities, using either the forward or the adjoint methods.

### 1.1 Historical Background

FORTRAN solvers for ODE initial value problems are widespread and heavily used. Two solvers that have been written at LLNL in the past are VODE [3] and VODPK [5]. 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 [30]. 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 [4]. The capabilities of both VODE and VODPK have been combined in the C-language package CVODE [10].

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) [33], FGMRES (Flexible Generalized Minimum RESidual) [32], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [36], TFQMR (Transpose-Free Quasi-Minimal Residual) [14], and PCG (Preconditioned Conjugate Gradient) [15] 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 PVODE [7], the parallel variant of CVODE.

CVODES is written with a functionality that is a superset of that of the pair CVODE/PVODE. Sensitivity analysis capabilities, both forward and adjoint, have been added to the main integrator. Enabling forward sensitivity computations in CVODES will result in the code integrating the so-called *sensitivity equations* simultaneously with the original IVP, yielding both the solution and its sensitivity with respect to parameters in the model. Adjoint sensitivity analysis, most useful when the gradients of relatively few functionals of the solution with respect to many parameters are sought, involves integration of the original IVP forward in time followed by the integration of the so-called *adjoint equations* backward in time. CVODES provides the infrastructure needed to integrate any final-condition ODE dependent on the solution of the original IVP (in particular the adjoint system).

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

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

## 1.2 Changes from previous versions

### Changes in 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 `boolean` type 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.

A bug was fixed in the interpolation functions used in solving backward problems for adjoint sensitivity analysis.

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

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

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

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

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

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

## Changes in v2.8.0

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

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

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

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

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

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

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

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

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

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

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

In the example `cvshessian_ASA_FSA`, an error was corrected in the function `fb2`: `y2` in place of `y3` in the third term of `Ith(yBdot,6)`.

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

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

## Changes in v2.7.0

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

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

A large number of minor errors have been fixed. Among these are the following: In `CVSetTqBDF`, the logic was changed to avoid a divide by zero. After the solver memory is created, it is set to zero before being filled. In each linear solver interface function, the linear solver memory is freed on an error return, and the `**Free` function now includes a line setting to NULL the main memory pointer to the linear solver memory. In the rootfinding functions `CVRcheck1/CVRcheck2`, when an exact zero is found, the array `glo` of  $g$  values at the left endpoint is adjusted, instead of shifting the  $t$  location `tlo` slightly. In the installation files, we modified the treatment of the macro `SUNDIALS_USE_GENERIC_MATH`, so that the parameter `GENERIC_MATH_LIB` is either defined (with no value) or not defined.

## Changes in v2.6.0

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

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

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

## Changes in v2.5.0

The main changes in this release involve a rearrangement of the entire SUNDIALS source tree (see §3.1). At the user interface level, the main impact is in the mechanism of including SUNDIALS header files which must now include the relative path (e.g. `#include <cvode/cvode.h>`). Additional changes

were made to the build system: all exported header files are now installed in separate subdirectories of the installation *include* directory.

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

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

## Changes in v2.4.0

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

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

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

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

## Changes in v2.3.0

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

## Changes in v2.2.0

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

## Changes in v2.1.2

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

## Changes in v2.1.1

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

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



## Changes in v2.1.0

The major changes from the previous version involve a redesign of the user interface across the entire SUNDIALS suite. We have eliminated the mechanism of providing optional inputs and extracting optional statistics from the solver through the `iopt` and `ropt` arrays. Instead, CVODES now provides a set of routines (with prefix `CVodeSet`) to change the default values for various quantities controlling the solver and a set of extraction routines (with prefix `CVodeGet`) to extract statistics after return from the main solver routine. Similarly, each linear solver module provides its own set of `Set`- and `Get`-type routines. For more details see §4.5.6 and §4.5.8.

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

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

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

## 1.3 Reading this User Guide

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

There are different possible levels of usage of CVODES. The most casual user, with a small IVP problem only, can get by with reading §2.1, then Chapter 4 through §4.5.5 only, and looking at examples in [35]. In addition, to solve a forward sensitivity problem the user should read §2.6, followed by Chapter 5 through §5.2.4 only, and look at examples in [35].

In a different direction, a more expert user with an IVP problem may want to (a) use a package preconditioner (§4.8), (b) supply his/her own Jacobian or preconditioner routines (§4.6), (c) do multiple runs of problems of the same size (§4.5.9), (d) supply a new NVECTOR module (Chapter 7), or even (e) supply new SUNLINSOL and/or SUNMATRIX modules (Chapters 8 and 9). An advanced user with a forward sensitivity problem may also want to (a) provide his/her own sensitivity equations right-hand side routine (§5.3), (b) perform multiple runs with the same number of sensitivity parameters (§5.2.1), or (c) extract additional diagnostic information (§5.2.4). A user with an adjoint sensitivity problem needs to understand the IVP solution approach at the desired level and also go through §2.7 for a short mathematical description of the adjoint approach, Chapter 6 for the usage of the adjoint module in CVODES, and the examples in [35].

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by CVODES for the solution of initial value problems for systems of ODEs, continue with short descriptions of preconditioning (§2.2), stability limit detection (§2.3), and rootfinding (§2.4), and conclude with an overview of the mathematical aspects of sensitivity analysis, both forward (§2.6) and adjoint (§2.7).
- The following chapter describes the structure of the SUNDIALS suite of solvers (§3.1) and the software organization of the CVODES solver (§3.2).
- Chapter 4 is the main usage document for CVODES for simulation applications. It includes a complete description of the user interface for the integration of ODE initial value problems. Readers that are not interested in using CVODES for sensitivity analysis can then skip the next two chapters.
- Chapter 5 describes the usage of CVODES for forward sensitivity analysis as an extension of its IVP integration capabilities. We begin with a skeleton of the user main program, with emphasis

on the steps that are required in addition to those already described in Chapter 4. Following that we provide detailed descriptions of the user-callable interface routines specific to forward sensitivity analysis and of the additional optional user-defined routines.

- Chapter 6 describes the usage of CVODES for adjoint sensitivity analysis. We begin by describing the CVODES checkpointing implementation for interpolation of the original IVP solution during integration of the adjoint system backward in time, and with an overview of a user's main program. Following that we provide complete descriptions of the user-callable interface routines for adjoint sensitivity analysis as well as descriptions of the required additional user-defined routines.
- Chapter 7 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 8 gives a brief overview of the generic SUNMATRIX module shared among the various components of SUNDIALS, and details on the SUNMATRIX implementations provided with SUNDIALS: a dense implementation (§8.1), a banded implementation (§8.2) and a sparse implementation (§8.3).
- Chapter 9 gives a brief overview of the generic SUNLINSOL module shared among the various components of SUNDIALS. This chapter contains details on the SUNLINSOL implementations provided with SUNDIALS. The chapter also contains details on the SUNLINSOL implementations provided with SUNDIALS that interface with external linear solver libraries.
- Finally, in the appendices, we provide detailed instructions for the installation of CVODES, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from CVODES functions (Appendix B).

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



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## Chapter 2

# Mathematical Considerations

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

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

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. CVODES solves both stiff and non-stiff systems. Roughly speaking, stiffness is characterized by the presence of at least one rapidly damped mode, whose time constant is small compared to the time scale of the solution itself.

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

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

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

### 2.1 IVP solution

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

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

Here the  $y^n$  are computed approximations to  $y(t_n)$ , and  $h_n = t_n - t_{n-1}$  is the step size. The user of CVODE must choose appropriately one of two multistep methods. For nonstiff problems, CVODE includes the Adams-Moulton formulas, characterized by  $K_1 = 1$  and  $K_2 = q$  above, where the order  $q$  varies between 1 and 12. For stiff problems, CVODES includes the Backward Differentiation Formulas (BDF) in so-called fixed-leading coefficient (FLC) form, given by  $K_1 = q$  and  $K_2 = 0$ , with order  $q$  varying between 1 and 5. The coefficients are uniquely determined by the method type, its order, the recent history of the step sizes, and the normalization  $\alpha_{n,0} = -1$ . See [6] and [25].

For either choice of formula, the nonlinear system

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

where  $a_n \equiv \sum_{i>0} (\alpha_{n,i} y^{n-i} + h_n \beta_{n,i} \dot{y}^{n-i})$ , must be solved (approximately) at each integration step. For this, CVODES offers the choice of either *functional iteration*, suitable only for nonstiff systems, and various versions of *Newton iteration*. Functional iteration, given by

$$y^{n(m+1)} = h_n \beta_{n,0} f(t_n, y^{n(m)}) + a_n,$$

involves evaluations of  $f$  only. In contrast, Newton iteration requires the solution of linear systems

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

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 initial guess for the iteration is a predicted value  $y^{n(0)}$  computed explicitly from the available history data.

For the solution of the linear systems within the Newton corrections, CVODES provides several choices, including the option of an user-supplied linear solver module. 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 [11, 1], or the thread-enabled SuperLU\_MT sparse solver library [27, 12, 2] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SUPERLUMT packages independent of CVODES],
- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver,
- SPFGMR, a scaled preconditioned FGMRES (Flexible Generalized Minimal Residual method) solver,
- SPBCGS, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver,
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver, or
- PCG, a scaled preconditioned CG (Conjugate Gradient method) solver.

For large stiff systems, where direct methods are 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 [4].

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

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

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

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

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 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. 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 stopping test for the Newton iteration is related to the subsequent local error test, with the goal of keeping the nonlinear iteration errors from interfering with local error control. As described below, the final computed value  $y^{n(m)}$  will have to satisfy a local error test  $\|y^{n(m)} - y^{n(0)}\| \leq \epsilon$ . Letting  $y^n$  denote the exact solution of (2.4), we want to ensure that the iteration error  $y^n - y^{n(m)}$  is small relative to  $\epsilon$ , 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 CVODES — making it an ODE “solver” rather than just an ODE method, is its control of local error. At every step, the local error is estimated and required to satisfy tolerance conditions, and the step is redone with reduced step size whenever that error test fails. As with any linear multistep method, the local truncation error LTE, at order  $q$  and step size  $h$ , satisfies an asymptotic relation

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

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

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

The local error test is simply  $\|\text{LTE}\| \leq 1$ . 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, CVODES returns to the user with a give-up message.

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

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

We consider changing order only after taking  $q+1$  steps at order  $q$ , and then we consider only orders  $q' = q-1$  (if  $q > 1$ ) or  $q' = q+1$  (if  $q < 5$ ). The local truncation error at order  $q'$  is estimated using the history data. Then a tentative step size ratio is computed on the basis that this error,  $\text{LTE}(q')$ , 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 CVODES described above, as inherited from VODE and VODPK, are documented in [3, 5, 19]. They are also summarized in [20].

Normally, CVODES 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 CVODES not to integrate past a given stopping point  $t = t_{\text{stop}}$ .

## 2.2 Preconditioning

When using a Newton method to solve the nonlinear system (2.4), CVODES makes repeated use of a linear solver to solve linear systems of the form  $Mx = -r$ , where  $x$  is a correction vector and  $r$  is a residual vector. If this linear system solve is done with one of the scaled preconditioned iterative linear solvers, these solvers are rarely successful if used without preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system  $Ax = b$  can be preconditioned on the left, as  $(P^{-1}A)x = P^{-1}b$ ; on the right, as  $(AP^{-1})Px = b$ ; or on both sides, as  $(P_L^{-1}AP_R^{-1})P_Rx = P_L^{-1}b$ . The Krylov method is then applied to a system with the matrix  $P^{-1}A$ , or  $AP^{-1}$ , or  $P_L^{-1}AP_R^{-1}$ , instead of  $A$ . In order to improve the convergence of the Krylov iteration, the preconditioner matrix  $P$ , or the product  $P_L P_R$  in the last case, should in some sense approximate the system matrix  $A$ . Yet at the same time, in order to be cost-effective, the matrix  $P$ , or matrices  $P_L$  and  $P_R$ , should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [4] for an extensive study of preconditioners for reaction-transport systems).

Most of the iterative linear solvers supplied with SUNDIALS allow for preconditioning either side, or on both sides, although we know of no situation where preconditioning on both sides is clearly superior to preconditioning on one side only (with the product  $P_L P_R$ ). Moreover, for a given preconditioner matrix, the merits of left vs. right preconditioning are unclear in general, and the user should experiment with both choices. Performance will differ because the inverse of the left preconditioner is included in the linear system residual whose norm is being tested in the Krylov algorithm. As a rule, however, if the preconditioner is the product of two matrices, we recommend that preconditioning be done either on the left only or the right only, rather than using one factor on each side.

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

## 2.3 BDF stability limit detection

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

When the BDF option is selected, CVODES uses Backward Differentiation Formula methods of orders 1 to 5. At order 1 or 2, the BDF method is A-stable, meaning that for any complex constant  $\lambda$  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 [17]. The algorithm supplements (but differs greatly from) the existing algorithms in CVODES for choosing step size and order based on estimated local truncation errors. The STALD algorithm works directly with history data that is readily available in CVODES. If it concludes that the step size is in fact stability-limited, it dictates a reduction in the method order, regardless of the outcome of the error-based algorithm. The STALD algorithm has been tested in combination with the VODE solver on linear advection-dominated advection-diffusion problems [18], where it works well. The implementation in CVODES has been successfully tested on linear and nonlinear advection-diffusion problems, among others.

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

## 2.4 Rootfinding

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

integration.

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

The basic scheme used is to check for sign changes of any  $g_i(t)$  over each time step taken, and then (when a sign change is found) to hone in on the root(s) with a modified secant method [16]. In addition, each time  $g$  is computed, CVODES checks to see if  $g_i(t) = 0$  exactly, and if so it reports this as a root. However, if an exact zero of any  $g_i$  is found at a point  $t$ , CVODES computes  $g$  at  $t + \delta$  for a small increment  $\delta$ , slightly further in the direction of integration, and if any  $g_i(t + \delta) = 0$  also, CVODES stops and reports an error. This way, each time CVODES takes a time step, it is guaranteed that the values of all  $g_i$  are nonzero at some past value of  $t$ , beyond which a search for roots is to be done.

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

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

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

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

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

where  $\alpha$  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  $\tau/2$ .

## 2.5 Pure quadrature integration

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

$$z(t) = \int_{t_0}^t q(\tau, y(\tau), p) d\tau . \quad (2.9)$$

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

$$\dot{z} = q(t, y, p), \quad z(t_0) = 0 . \quad (2.10)$$

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

This can be done at the “user level” by simply exposing to CVODES the extended ODE system (2.2)+(2.9). However, in the context of an implicit integration solver, this approach is not desirable since the nonlinear solver module will require the Jacobian (or Jacobian-vector product) of this extended ODE. Moreover, since the additional states  $z$  do not enter the right-hand side of the ODE (2.9) and therefore the right-hand side of the extended ODE system, it is much more efficient to treat the ODE system (2.9) separately from the original system (2.2) by “taking out” the additional states  $z$  from the nonlinear system (2.4) that must be solved in the correction step of the LMM. Instead, “corrected” values  $z^n$  are computed explicitly as

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

once the new approximation  $y^n$  is available.

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

## 2.6 Forward sensitivity analysis

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

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

$$\dot{s}_i = \frac{\partial f}{\partial y} s_i + \frac{\partial f}{\partial p_i}, \quad s_i(t_0) = \frac{\partial y_0(p)}{\partial p_i}, \quad (2.11)$$

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

When performing forward sensitivity analysis, CVODES carries out the time integration of the combined system, (2.2) and (2.11), by viewing it as an ODE system of size  $N(N_s + 1)$ , where  $N_s$  is the number of model parameters  $p_i$ , with respect to which sensitivities are desired ( $N_s \leq N_p$ ). However, major improvements in efficiency can be made by taking advantage of the special form of the sensitivity equations as linearizations of the original ODEs. In particular, for stiff systems, for which CVODES employs a Newton iteration, the original ODE system and all sensitivity systems share the same Jacobian matrix, and therefore the same iteration matrix  $M$  in (2.6).

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

### 2.6.1 Forward sensitivity methods

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

- *Staggered Direct*

In this approach [9], the nonlinear system (2.4) is first solved and, once an acceptable numerical solution is obtained, the sensitivity variables at the new step are found by directly solving (2.11) after the (BDF or Adams) discretization is used to eliminate  $\dot{s}_i$ . Although the system matrix

of the above linear system is based on exactly the same information as the matrix  $M$  in (2.6), it must be updated and factored at every step of the integration, in contrast to an evaluation of  $M$  which is updated only occasionally. For problems with many parameters (relative to the problem size), the staggered direct method can outperform the methods described below [26]. However, the computational cost associated with matrix updates and factorizations makes this method unattractive for problems with many more states than parameters (such as those arising from semidiscretization of PDEs) and is therefore not implemented in CVODES.

- *Simultaneous Corrector*

In this method [28], the discretization is applied simultaneously to both the original equations (2.2) and the sensitivity systems (2.11) resulting in the following nonlinear system

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

where  $\hat{f} = [f(t, y, p), \dots, (\partial f / \partial y)(t, y, p) s_i + (\partial f / \partial p_i)(t, y, p), \dots]$ , and  $\hat{a}_n$  is comprised of the terms in the discretization that depend on the solution at previous integration steps. This combined nonlinear system can be solved using a modified Newton method as in (2.5) by solving the corrector equation

$$\hat{M}[\hat{y}_{n(m+1)} - \hat{y}_{n(m)}] = -\hat{G}(\hat{y}_{n(m)}) \quad (2.12)$$

at each iteration, where

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

$M$  is defined as in (2.6), and  $J_i = (\partial / \partial y) [(\partial f / \partial y) s_i + (\partial f / \partial p_i)]$ . It can be shown that 2-step quadratic convergence can be retained by using only the block-diagonal portion of  $\hat{M}$  in the corrector equation (2.12). This results in a decoupling that allows the reuse of  $M$  without additional matrix factorizations. However, the products  $(\partial f / \partial y) s_i$  and the vectors  $\partial f / \partial p_i$  must still be reevaluated at each step of the iterative process (2.12) to update the sensitivity portions of the residual  $\hat{G}$ .

- *Staggered corrector*

In this approach [13], as in the staggered direct method, the nonlinear system (2.4) is solved first using the Newton iteration (2.5). Then a separate Newton iteration is used to solve the sensitivity system (2.11):

$$M[s_i^{n(m+1)} - s_i^{n(m)}] = - \left[ s_i^{n(m)} - \gamma \left( \frac{\partial f}{\partial y}(t_n, y^n, p) s_i^{n(m)} + \frac{\partial f}{\partial p_i}(t_n, y^n, p) \right) - a_{i,n} \right], \quad (2.13)$$

where  $a_{i,n} = \sum_{j>0} (\alpha_{n,j} s_i^{n-j} + h_n \beta_{n,j} \dot{s}_i^{n-j})$ . In other words, a modified Newton iteration is used to solve a linear system. In this approach, the vectors  $\partial f / \partial p_i$  need be updated only once per integration step, after the state correction phase (2.5) has converged. Note also that Jacobian-related data can be reused at all iterations (2.13) to evaluate the products  $(\partial f / \partial y) s_i$ .

CVODES implements the simultaneous corrector method and two flavors of the staggered corrector method which differ only if the sensitivity variables are included in the error control test. In the *full error control* case, the first variant of the staggered corrector method requires the convergence of the iterations (2.13) for all  $N_s$  sensitivity systems and then performs the error test on the sensitivity variables. The second variant of the method will perform the error test for each sensitivity vector  $s_i, (i = 1, 2, \dots, N_s)$  individually, as they pass the convergence test. Differences in performance

between the two variants may therefore be noticed whenever one of the sensitivity vectors  $s_i$  fails a convergence or error test.

An important observation is that the staggered corrector method, combined with a Krylov linear solver, effectively results in a staggered direct method. Indeed, the Krylov solver requires only the action of the matrix  $M$  on a vector and this can be provided with the current Jacobian information. Therefore, the modified Newton procedure (2.13) will theoretically converge after one iteration.

### 2.6.2 Selection of the absolute tolerances for sensitivity variables

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

### 2.6.3 Evaluation of the sensitivity right-hand side

There are several methods for evaluating the right-hand side of the sensitivity systems (2.11): analytic evaluation, automatic differentiation, complex-step approximation, and finite differences (or directional derivatives). CVODES provides all the software hooks for implementing interfaces to automatic differentiation (AD) or complex-step approximation; future versions will include a generic interface to AD-generated functions. At the present time, besides the option for analytical sensitivity right-hand sides (user-provided), CVODES can evaluate these quantities using various finite difference-based approximations to evaluate the terms  $(\partial f/\partial y)s_i$  and  $(\partial f/\partial p_i)$ , or using directional derivatives to evaluate  $[(\partial f/\partial y)s_i + (\partial f/\partial p_i)]$ . As is typical for finite differences, the proper choice of perturbations is a delicate matter. CVODES takes into account several problem-related features: the relative ODE error tolerance  $\text{RTOL}$ , the machine unit roundoff  $U$ , the scale factor  $\bar{p}_i$ , and the weighted root-mean-square norm of the sensitivity vector  $s_i$ .

Using central finite differences as an example, the two terms  $(\partial f/\partial y)s_i$  and  $\partial f/\partial p_i$  in the right-hand side of (2.11) can be evaluated either separately:

$$\frac{\partial f}{\partial y}s_i \approx \frac{f(t, y + \sigma_y s_i, p) - f(t, y - \sigma_y s_i, p)}{2\sigma_y}, \quad (2.14)$$

$$\frac{\partial f}{\partial p_i} \approx \frac{f(t, y, p + \sigma_i e_i) - f(t, y, p - \sigma_i e_i)}{2\sigma_i}, \quad (2.14')$$

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

or simultaneously:

$$\frac{\partial f}{\partial y}s_i + \frac{\partial f}{\partial p_i} \approx \frac{f(t, y + \sigma s_i, p + \sigma e_i) - f(t, y - \sigma s_i, p - \sigma e_i)}{2\sigma}, \quad (2.15)$$

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

or by adaptively switching between (2.14)+(2.14') and (2.15), depending on the relative size of the finite difference increments  $\sigma_i$  and  $\sigma_y$ . In the adaptive scheme, if  $\rho = \max(\sigma_i/\sigma_y, \sigma_y/\sigma_i)$ , we use separate evaluations if  $\rho > \rho_{\max}$  (an input value), and simultaneous evaluations otherwise.



These procedures for choosing the perturbations  $(\sigma_i, \sigma_y, \sigma)$  and switching between finite difference and directional derivative formulas have also been implemented for one-sided difference formulas. Forward finite differences can be applied to  $(\partial f / \partial y) s_i$  and  $\partial f / \partial p_i$  separately, or the single directional derivative formula

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

can be used. In CVODES, the default value of  $\rho_{\max} = 0$  indicates the use of the second-order centered directional derivative formula (2.15) exclusively. Otherwise, the magnitude of  $\rho_{\max}$  and its sign (positive or negative) indicates whether this switching is done with regard to (centered or forward) finite differences, respectively.

### 2.6.4 Quadratures depending on forward sensitivities

If pure quadrature variables are also included in the problem definition (see §2.5), CVODES does *not* carry their sensitivities automatically. Instead, we provide a more general feature through which integrals depending on both the states  $y$  of (2.2) and the state sensitivities  $s_i$  of (2.11) can be evaluated. In other words, CVODES provides support for computing integrals of the form:

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

If the sensitivities of the quadrature variables  $z$  of (2.9) are desired, these can then be computed by using:

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

as integrands for  $\bar{z}$ , where  $q_y$  and  $q_p$  are the partial derivatives of the integrand function  $q$  of (2.9).

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

## 2.7 Adjoint sensitivity analysis

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

$$G(p) = \int_{t_0}^T g(t, y, p) dt, \tag{2.16}$$

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

In what follows, we only sketch the analysis for the sensitivity problem for both  $G$  and  $g$ . For details on the derivation see [8]. Introducing a Lagrange multiplier  $\lambda$ , we form the augmented objective function

$$I(p) = G(p) - \int_{t_0}^T \lambda^* (\dot{y} - f(t, y, p)) dt, \tag{2.17}$$

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

$$\frac{dG}{dp} = \frac{dI}{dp} = \int_{t_0}^T (g_p + g_y s) dt - \int_{t_0}^T \lambda^* (\dot{s} - f_y s - f_p) dt, \tag{2.18}$$

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

$$\begin{aligned}\dot{\lambda} &= - \left( \frac{\partial f}{\partial y} \right)^* \lambda - \left( \frac{\partial g}{\partial y} \right)^* \\ \lambda(T) &= 0,\end{aligned}\tag{2.19}$$

the gradient of  $G$  with respect to  $p$  is nothing but

$$\frac{dG}{dp} = \lambda^*(t_0)s(t_0) + \int_{t_0}^T (g_p + \lambda^* f_p) dt.\tag{2.20}$$

The gradient of  $g(T, y, p)$  with respect to  $p$  can be then obtained by using the Leibnitz differentiation rule. Indeed, from (2.16),

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

and therefore, taking into account that  $dG/dp$  in (2.20) depends on  $T$  both through the upper integration limit and through  $\lambda$ , and that  $\lambda(T) = 0$ ,

$$\frac{dg}{dp}(T) = \mu^*(t_0)s(t_0) + g_p(T) + \int_{t_0}^T \mu^* f_p dt,\tag{2.21}$$

where  $\mu$  is the sensitivity of  $\lambda$  with respect to the final integration limit  $T$ . Thus  $\mu$  satisfies the following equation, obtained by taking the total derivative with respect to  $T$  of (2.19):

$$\begin{aligned}\dot{\mu} &= - \left( \frac{\partial f}{\partial y} \right)^* \mu \\ \mu(T) &= \left( \frac{\partial g}{\partial y} \right)^*_{t=T}.\end{aligned}\tag{2.22}$$

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

The first thing to notice about the adjoint system (2.19) is that there is no explicit specification of the parameters  $p$ ; this implies that, once the solution  $\lambda$  is found, the formula (2.20) can then be used to find the gradient of  $G$  with respect to any of the parameters  $p$ . The same holds true for the system (2.22) and the formula (2.21) for gradients of  $g(T, y, p)$ . The second important remark is that the adjoint systems (2.19) and (2.22) are terminal value problems which depend on the solution  $y(t)$  of the original IVP (2.2). Therefore, a procedure is needed for providing the states  $y$  obtained during a forward integration phase of (2.2) to CVODES during the backward integration phase of (2.19) or (2.22). The approach adopted in CVODES, based on *checkpointing*, is described below.

### 2.7.1 Checkpointing scheme

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

However, especially for large-scale problems and long integration intervals, the number and size of the vectors  $y$  and  $\dot{y}$  that would need to be stored make this approach computationally intractable.



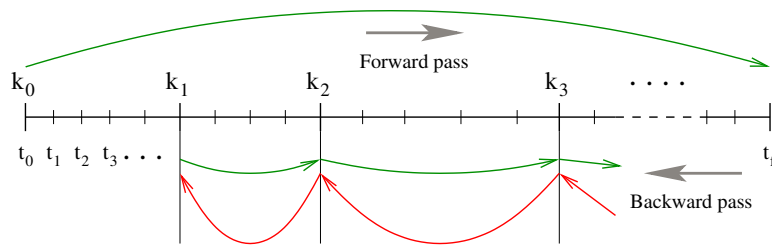


Figure 2.1: Illustration of the checkpointing algorithm for generation of the forward solution during the integration of the adjoint system.

Thus, CVODES settles for a compromise between storage space and execution time by implementing a so-called *checkpointing scheme*. At the cost of at most one additional forward integration, this approach offers the best possible estimate of memory requirements for adjoint sensitivity analysis. To begin with, based on the problem size  $N$  and the available memory, the user decides on the number  $N_d$  of data pairs  $(y, \dot{y})$  if cubic Hermite interpolation is selected, or on the number  $N_d$  of  $y$  vectors in the case of variable-degree polynomial interpolation, that can be kept in memory for the purpose of interpolation. Then, during the first forward integration stage, after every  $N_d$  integration steps a checkpoint is formed by saving enough information (either in memory or on disk) to allow for a hot restart, that is a restart which will exactly reproduce the forward integration. In order to avoid storing Jacobian-related data at each checkpoint, a reevaluation of the iteration matrix is forced before each checkpoint. At the end of this stage, we are left with  $N_c$  checkpoints, including one at  $t_0$ . During the backward integration stage, the adjoint variables are integrated from  $T$  to  $t_0$  going from one checkpoint to the previous one. The backward integration from checkpoint  $i + 1$  to checkpoint  $i$  is preceded by a forward integration from  $i$  to  $i + 1$  during which the  $N_d$  vectors  $y$  (and, if necessary  $\dot{y}$ ) are generated and stored in memory for interpolation<sup>1</sup> (see Fig. 2.1).

This approach transfers the uncertainty in the number of integration steps in the forward integration phase to uncertainty in the final number of checkpoints. However,  $N_c$  is much smaller than the number of steps taken during the forward integration, and there is no major penalty for writing/reading the checkpoint data to/from a temporary file. Note that, at the end of the first forward integration stage, interpolation data are available from the last checkpoint to the end of the interval of integration. If no checkpoints are necessary ( $N_d$  is larger than the number of integration steps taken in the solution of (2.2)), the total cost of an adjoint sensitivity computation can be as low as one forward plus one backward integration. In addition, CVODES provides the capability of reusing a set of checkpoints for multiple backward integrations, thus allowing for efficient computation of gradients of several functionals (2.16).

Finally, we note that the adjoint sensitivity module in CVODES provides the necessary infrastructure to integrate backwards in time any ODE terminal value problem dependent on the solution of the IVP (2.2), including adjoint systems (2.19) or (2.22), as well as any other quadrature ODEs that may be needed in evaluating the integrals in (2.20) or (2.21). In particular, for ODE systems arising from semi-discretization of time-dependent PDEs, this feature allows for integration of either the discretized adjoint PDE system or the adjoint of the discretized PDE.

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

The Hermite cubic interpolation option is present because it was implemented chronologically first and it is also used by other adjoint solvers (e.g. DASPKADJOINT). The variable-degree polynomial is more memory-efficient (it requires only half of the memory storage of the cubic Hermite interpolation) and is more accurate. The accuracy differences are minor when using BDF (since the maximum method order cannot exceed 5), but can be significant for the Adams method for which the order can reach 12.

## 2.8 Second-order sensitivity analysis

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

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

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

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

where  $y_p$  is the first-order sensitivity matrix, the solution of  $N_p$  systems (2.11), and  $y_{pp}$  is a third-order tensor. It is easy to see that, except for situations in which the number of parameters  $N_p$  is very small, the computational cost of this so-called *forward-over-forward* approach is exorbitant as it requires the solution of  $N_p + N_p^2$  additional ODE systems of the same dimension  $N$  as (2.2).

A much more efficient alternative is to compute Hessian-vector products using a so-called *forward-over-adjoint* approach. This method is based on using the same “trick” as the one used in computing gradients of pointwise functionals with the adjoint method, namely applying a formal directional forward derivation to one of the gradients of (2.20) or (2.21). With that, the cost of computing a full Hessian is roughly equivalent to the cost of computing the gradient with forward sensitivity analysis. However, Hessian-vector products can be cheaply computed with one additional adjoint solve. Consider for example,  $G(p) = \int_{t_0}^{t_f} g(t, y) dt$ . It can be shown that the product between the Hessian of  $G$  (with respect to the parameters  $p$ ) and some vector  $u$  can be computed as

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

where  $\lambda$ ,  $\mu$ , and  $s$  are solutions of

$$\begin{aligned} -\dot{\mu} &= f_y^T \mu + (\lambda^T \otimes I_n) f_{yy} s + g_{yy} s; & \mu(t_f) &= 0 \\ -\dot{\lambda} &= f_y^T \lambda + g_y^T; & \lambda(t_f) &= 0 \\ \dot{s} &= f_y s; & s(t_0) &= y_{0p} u \end{aligned} \tag{2.23}$$

In the above equation,  $s = y_p u$  is a linear combination of the columns of the sensitivity matrix  $y_p$ . The *forward-over-adjoint* approach hinges crucially on the fact that  $s$  can be computed at the cost of a forward sensitivity analysis with respect to a single parameter (the last ODE problem above) which is possible due to the linearity of the forward sensitivity equations (2.11).

Therefore, the cost of computing the Hessian-vector product is roughly that of two forward and two backward integrations of a system of ODEs of size  $N$ . For more details, including the corresponding formulas for a pointwise model functional output, see [29].

To allow the *forward-over-adjoint* approach described above, CVODES provides support for:

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

<sup>2</sup>For the sake of simplifty in presentation, we do not include explicit dependencies of  $g$  on time  $t$  or parameters  $p$ . Moreover, we only consider the case in which the dependency of the original ODE (2.2) on the parameters  $p$  is through its initial conditions only. For details on the derivation in the general case, see [29].

## 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 Fig. 3.1). The following is a list of the solver packages presently available, and the basic functionality of each:

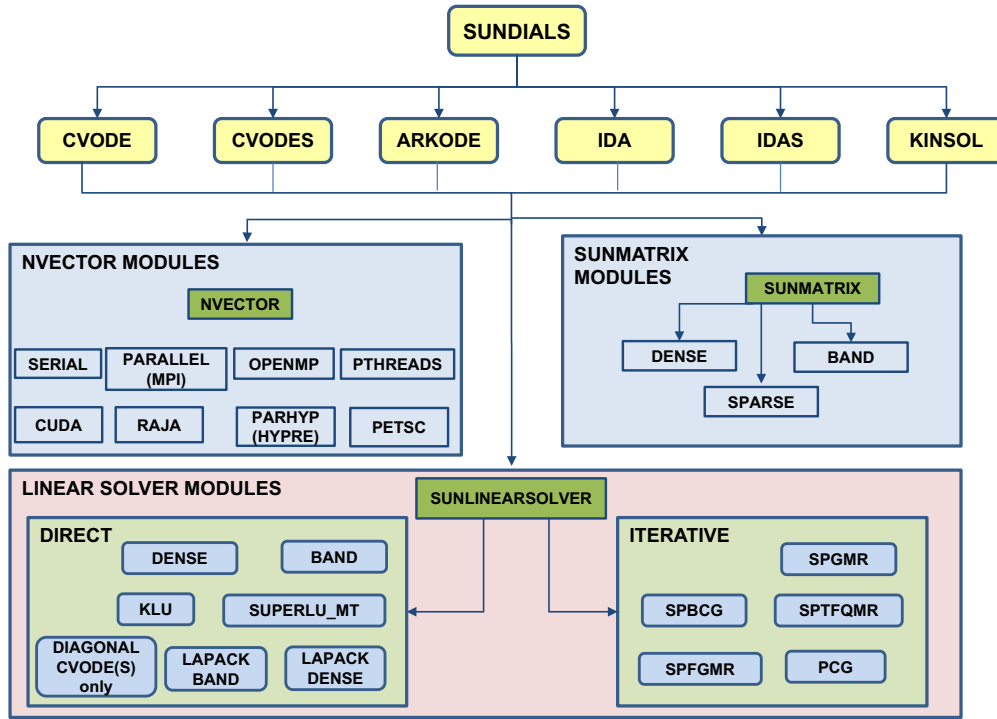
- CVODE, a solver for stiff and nonstiff ODE systems  $dy/dt = f(t, y)$  based on Adams and BDF methods;
- CVODES, a solver for stiff and nonstiff ODE systems with sensitivity analysis capabilities;
- ARKODE, a solver for ODE systems  $Mdy/dt = f_E(t, y) + f_I(t, y)$  based on additive Runge-Kutta methods;
- 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 CVODES organization

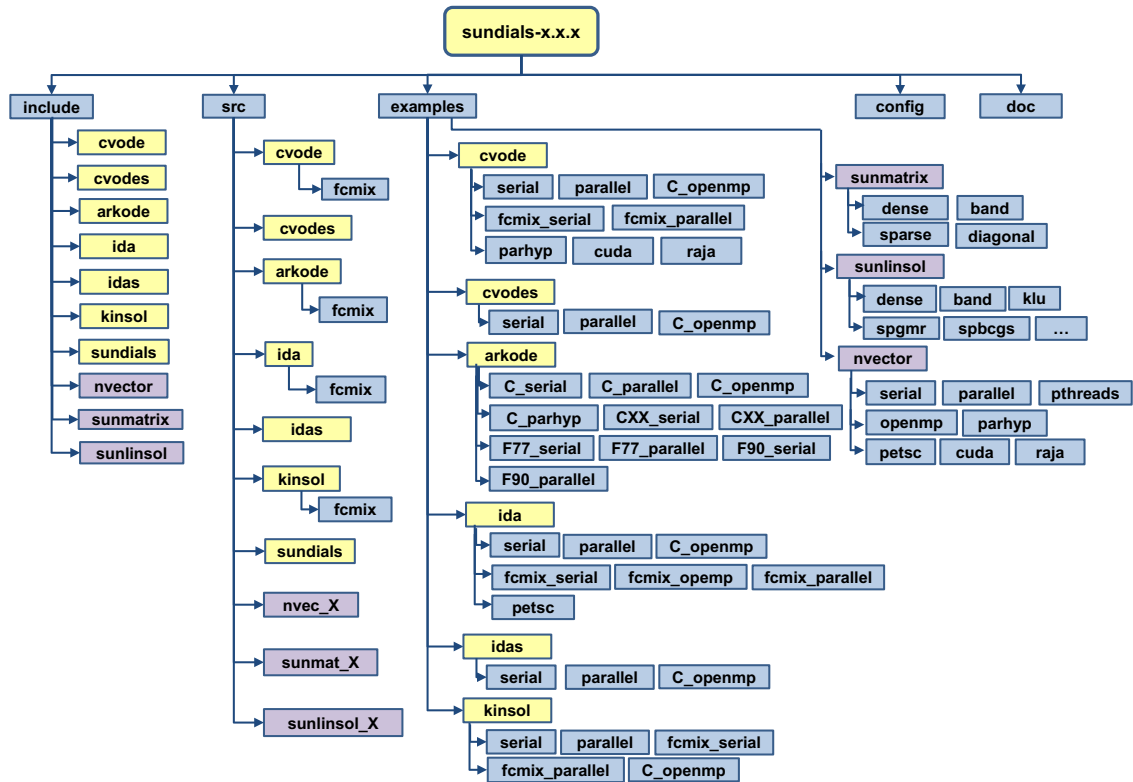
The CVODES package is written in ANSI C. The following summarizes the basic structure of the package, although knowledge of this structure is not necessary for its use.

The overall organization of the CVODES package is shown in Figure 3.2. The basic elements of the structure are a module for the basic integration algorithm (including forward sensitivity analysis), a module for adjoint sensitivity analysis, and support for the solution of linear systems that arise in the case of a stiff system. The central integration module, implemented in the files `cvode.h`, `cvode_impl.h`, and `cvode.c`, deals with the evaluation of integration coefficients, the functional or Newton iteration process, estimation of local error, selection of stepsize and order, and interpolation to user output points, among other issues. Although this module contains logic for the basic Newton iteration algorithm, it has no knowledge of the method being used to solve the linear systems that arise. For any given user problem, one of the linear system solver interfaces is specified, and is then invoked as needed during the integration.

In addition, if forward sensitivity analysis is turned on, the main module will integrate the forward sensitivity equations simultaneously with the original IVP. The sensitivity variables may be included in the local error control mechanism of the main integrator. CVODES provides three different strategies



(a) High-level diagram



(b) Directory structure of the source tree

Figure 3.1: Organization of the SUNDIALS suite

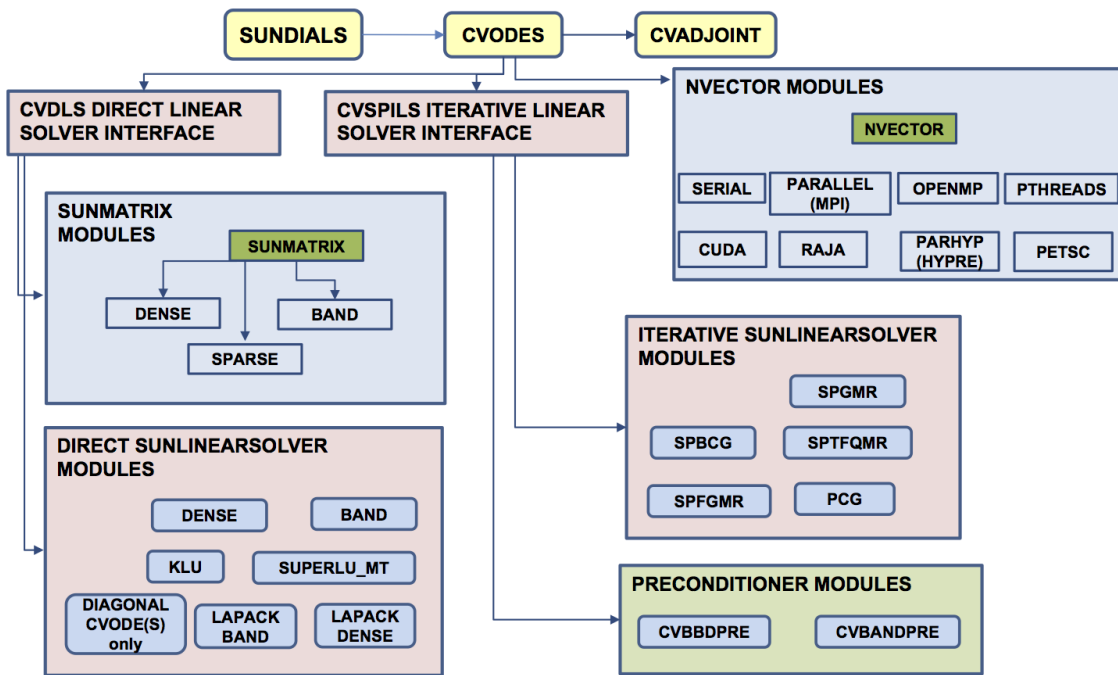


Figure 3.2: Overall structure of the CVODES package. Modules specific to CVODES begin with “CV” (CVDLS, CVSPILS, CVBBDPRE and CVBANDPRE), all other items correspond to generic solver and auxiliary modules. Note also that the LAPACK, KLU and SUPERLUMT support is through interfaces to external packages. Users will need to download and compile those packages independently.

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

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

At present, the package includes two linear solver interfaces. The *direct* linear solver interface, `CVDLS`, supports `SUNLINSOL` implementations with type `SUNLINSOL_DIRECT` (see Chapter 9). 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 8). It is assumed that the dominant cost for such solvers occurs in factorization of the linear system matrix  $M$ , so `CVODE` utilizes these solvers within its modified Newton nonlinear solve. The *spils* linear solver interface, `CVSPILS`, supports `SUNLINSOL` implementations with type `SUNLINSOL_ITERATIVE` (see Chapter 9). 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 `CVODES` will expand as new `SUNLINSOL` modules are developed.

Additionally, `CVODES` 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 [4, 5], together with the example and demonstration programs included with `CVODES`, 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.

`CVODES` also provides two preconditioner modules, for use with any of the Krylov iterative linear solvers. The first one, `CVBANDPRE`, is intended to be used with `NVECTOR_SERIAL`, `NVECTOR_OPENMP` or `NVECTOR_PTHREADS` and provides a banded difference-quotient Jacobian-based preconditioner, with corresponding setup and solve routines. The second preconditioner module, `CVBBDPRE`, works in conjunction with `NVECTOR_PARALLEL` and generates a preconditioner that is a block-diagonal matrix with each block being a banded matrix.

All state information used by `CVODES` to solve a given problem is saved in a structure, and a pointer to that structure is returned to the user. There is no global data in the `CVODES` package, and so, in this respect, it is reentrant. State information specific to the linear solver is saved in a separate structure, a pointer to which resides in the `CVODES` memory structure. The reentrancy of `CVODES` was motivated by the anticipated multicomputer extension, but is also essential in a uniprocessor setting where two or more problems are solved by intermixed calls to the package from within a single user program.

## Chapter 4

# Using CVODES for IVP Solution

This chapter is concerned with the use of CVODES for the solution of initial value problems (IVPs). The following sections treat the header files and the layout of the user's main program, and provide descriptions of the CVODES user-callable functions and user-supplied functions. This usage is essentially equivalent to using CVODE [21].

The sample programs described in the companion document [35] may also be helpful. Those codes may be used as templates (with the removal of some lines used in testing) and are included in the CVODES package.

The user should be aware that not all SUNLINSOL and SUNMATRIX modules are compatible with all NVECTOR implementations. Details on compatability are given in the documentation for each SUNMATRIX module (Chapter 8) and each SUNLINSOL module (Chapter 9). For example, NVECTOR\_PARALLEL is not compatible with the dense, banded, or sparse SUNMATRIX types, or with the corresponding dense, banded, or sparse SUNLINSOL modules. Please check Chapters 8 and 9 to verify 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.

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

### 4.1 Access to library and header files

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

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

- *libdir/libsundials\_cvodes.lib*,
- *libdir/libsundials\_nvec\*.lib* (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/cvodes*
- *incdir/include/sundials*
- *incdir/include/nvector*

- `incdir/include/sunmatrix`
- `incdir/include/sunlinsol`

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

Note that an application cannot link to both the `CVODE` and `CVODES` libraries because both contain user-callable functions with the same names (to ensure that `CVODES` is backward compatible with `CVODE`). Therefore, applications that contain both ODE problems and ODEs with sensitivity analysis, should use `CVODES`.

## 4.2 Data Types

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

### 4.2.1 Floating point types

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

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

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

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

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

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:

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

Note that `cvodes.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 an NVECTOR implementation header file, of the form `nvector/nvector_***.h`. See Chapter 7 for the appropriate name. This file in turn includes the header file `sundials_nvector.h` which defines the abstract `N_Vector` data type.

If the user chooses Newton iteration for the solution of the nonlinear systems, 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 CVODES are:

- `cvodes/cvodes_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`;
- `cvodes/cvodes_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_spgcrs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver module, `SUNLINSOL_SPGCRS`;
  - `sunlinsol/sunlinsol_sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov linear solver module, `SUNLINSOL_SPTFQMR`;

- `sunlinsol/sunlinsol_pcg.h`, which is used with the scaled, preconditioned CG Krylov linear solver module, `SUNLINSOL_PCG`;
- `cvodes/cvodes_diag.h`, which is used with the `CVDIAG` diagonal linear solver 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 `cvSdiurnal_kry_p` example (see [35]), 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 7, 8, and 9 for the specific name of the function to be called or macro to be referenced.

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

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

### 2. Set problem dimensions etc.

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

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

### 3. Set vector of initial values

To set the vector `y0` of initial values, use the appropriate functions defined by the particular `NVECTOR` implementation.

For native `SUNDIALS` vector implementations (except the `CUDA` and `RAJA`-based ones), use a call of the form `y0 = N_VMake_***(..., ydata)` if the `realtype` array `ydata` containing the initial values of  $y$  already exists. Otherwise, create a new vector by making a call of the form `y0 = N_VNew_***(...)`, and then set its elements by accessing the underlying data with a call of the form `ydata = N_VGetArrayPointer(y0)`. See §7.1-7.4 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 `hypr` or `PETSc` vector. Note that calls like `N_VNew_***(...)` and `N_VGetArrayPointer(...)` are not available for these vector wrappers. See §7.5 and §7.6 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 §7.7-7.8 for details.

#### 4. Create CVODES object

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

#### 5. Initialize CVODES solver

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

#### 6. Specify integration tolerances

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

#### 7. Set optional inputs

Call `CVodeSet*` functions to change any optional inputs that control the behavior of CVODES from their default values. See §4.5.6.1 for details.

#### 8. Create matrix object

If a direct linear solver is to be used within a Newton iteration then a template Jacobian matrix must be created by using the appropriate functions 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 Newton iteration is chosen, then the desired linear solver object must be created by using the appropriate functions 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 9 for details.

#### 11. Attach linear solver module

If a Newton iteration is chosen, 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 CVODES-specific diagonal linear solver module, CVDIAG, is desired, initialize the linear solver module and attach it to CVODES 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 §4.5.6 for details.

### 13. Specify rootfinding problem

Optionally, call `CVodeRootInit` to initialize a rootfinding problem to be solved during the integration of the ODE system. See §4.5.4, and see §4.5.6.4 for relevant optional input calls.

### 14. 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 §4.5.5 for details.

### 15. Get optional outputs

Call `CV*Get*` functions to obtain optional output. See §4.5.8 for details.

### 16. 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);
```

### 17. Free solver memory

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

### 18. Free linear solver and matrix memory

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

### 19. Finalize MPI, if used

Call `MPI_Finalize()` to terminate MPI.

SUNDIALS provides some linear solvers only as a means for users to get problems running and not as highly efficient solvers. For example, if solving a dense system, we suggest using the Lapack solvers if the size of the linear system is  $> 50,000$ . (Thanks to A. Nicolai for his testing and recommendation.) Table 4.1 shows the linear solver interfaces available as `SUNLINSOL` modules and the vector implementations required for use. As an example, one cannot use the dense direct solver interfaces with the MPI-based vector implementation. However, as discussed in Chapter 9 the SUNDIALS packages operate on generic `SUNLINSOL` objects, allowing a user to develop their own solvers should they so desire.

## 4.5 User-callable functions

This section describes the CVODES functions that are called by the user to setup and then solve an IVP. Some of these are required. However, starting with §4.5.6, the functions listed involve optional inputs/outputs or restarting, and those paragraphs may be skipped for a casual use of CVODES. In any case, refer to §4.4 for the correct order of these calls.

On an error, each user-callable function returns a negative value and sends an error message to the error handler routine, which prints the message on `stderr` by default. However, the user can set a file as error output or can provide his own error handler function (see §4.5.6.1).

### 4.5.1 CVODES initialization and deallocation functions

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

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.    | ✓      | ✓              | ✓      | ✓        | ✓    | ✓     | ✓    | ✓    | ✓          |

two calls.

#### CVodeCreate

Call `cvode_mem = CVodeCreate(lmm, iter);`

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

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

`iter` (`int`) specifies the type of nonlinear solver iteration and may be either `CV_NEWTON` or `CV_FUNCTIONAL`.

The recommended choices for `(lmm, iter)` are `(CV_ADAMS, CV_FUNCTIONAL)` for nonstiff problems and `(CV_BDF, CV_NEWTON)` for stiff problems.

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

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

`f` (`CVRhsFn`) is the C function which computes the right-hand side function  $f$  in the ODE. This function has the form `f(t, y, ydot, user_data)` (for full details see §4.6.1).

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

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

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

`CV_SUCCESS` The call to `CVodeInit` was successful.

`CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.

**CV\_MEM\_FAIL** A memory allocation request has failed.  
**CV\_ILL\_INPUT** An input argument to **CVodeInit** has an illegal value.  
 Notes If an error occurred, **CVodeInit** also sends an error message to the error handler function.

#### **CVodeFree**

Call `CVodeFree(&cvmem);`  
 Description The function **CVodeFree** frees the memory allocated by a previous call to **CVodeCreate**.  
 Arguments The argument is the pointer to the CVODES memory block (of type `void *`).  
 Return value The function **CVodeFree** has no return value.

### 4.5.2 CVODES tolerance specification functions

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

#### **CVodeSStolerances**

Call `flag = CVodeSStolerances(cvmem, reltol, abstol);`  
 Description The function **CVodeSStolerances** specifies scalar relative and absolute tolerances.  
 Arguments `cvmem` (`void *`) pointer to the CVODES memory block returned by **CVodeCreate**.  
     `reltol` (`realtype`) is the scalar relative error tolerance.  
     `abstol` (`realtype`) is the scalar absolute error tolerance.  
 Return value The return value `flag` (of type `int`) will be one of the following:  
     **CV\_SUCCESS** The call to **CVodeSStolerances** was successful.  
     **CV\_MEM\_NULL** The CVODES memory block was not initialized through a previous call to **CVodeCreate**.  
     **CV\_NO\_MALLOC** The allocation function **CVodeInit** has not been called.  
     **CV\_ILL\_INPUT** One of the input tolerances was negative.

#### **CVodeSVtolerances**

Call `flag = CVodeSVtolerances(cvmem, reltol, abstol);`  
 Description The function **CVodeSVtolerances** specifies scalar relative tolerance and vector absolute tolerances.  
 Arguments `cvmem` (`void *`) pointer to the CVODES memory block returned by **CVodeCreate**.  
     `reltol` (`realtype`) is the scalar relative error tolerance.  
     `abstol` (`N_Vector`) is the vector of absolute error tolerances.  
 Return value The return value `flag` (of type `int`) will be one of the following:  
     **CV\_SUCCESS** The call to **CVodeSVtolerances** was successful.  
     **CV\_MEM\_NULL** The CVODES memory block was not initialized through a previous call to **CVodeCreate**.  
     **CV\_NO\_MALLOC** The allocation function **CVodeInit** has not been called.  
     **CV\_ILL\_INPUT** The relative error tolerance was negative or the absolute tolerance had a negative component.  
 Notes This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the state vector  $y$ .

**CVodeWftolerances**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeWftolerances(cvode_mem, efun);</code>   |
| Description  | The function <code>CVodeWftolerances</code> specifies a user-supplied function <code>efun</code> that sets the multiplicative error weights $W_i$ for use in the weighted RMS norm, which are normally defined by Eq. (2.7).  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block returned by <code>CVodeCreate</code> .<br><code>efun</code> ( <code>CVEwtFn</code> ) is the C function which defines the <code>ewt</code> vector (see §4.6.3).  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <ul style="list-style-type: none"> <li><code>CV_SUCCESS</code> The call to <code>CVodeWftolerances</code> was successful.</li> <li><code>CV_MEM_NULL</code> The CVODES memory block was not initialized through a previous call to <code>CVodeCreate</code>.</li> <li><code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called.</li> </ul> |

**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 `cv Roberts_dns` in the CVODES package, and the discussion of it in the CVODES Examples document [35]. 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 CVODES, with magnitude comparable to `abstol` or less, is equivalent to zero as far as the computation is concerned.

(3) The user's right-hand side routine `f` should never change a negative value in the solution vector `y` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `f` routine cannot tolerate a zero or negative value (e.g. because there is a square root or log of it), then the



offending value should be changed to zero or a tiny positive number in a temporary variable (not in the input  $y$  vector) for the purposes of computing  $f(t, y)$ .

(4) Positivity and non-negativity constraints on components can be enforced by use of the recoverable error return feature in the user-supplied right-hand side function. However, because this option involves some extra overhead cost, it should only be exercised if the use of absolute tolerances to control the computed values is unsuccessful.

### 4.5.3 Linear solver interface functions

As previously explained, a Newton iteration requires the solution of linear systems of the form (2.5). There are three CVODES 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 Newton 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 Newton 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 §4.5.6 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 Newton matrix  $M = I - \gamma J$  of (2.6).

To specify a generic linear solver to CVODES, after the call to `CVodeCreate` but before any calls to `CVodes`, the user's program must create the appropriate SUNLINSOL object and call either of the functions `CVDlsSetLinearSolver` or `CVSpilsSetLinearSolver`, as documented below. The first argument passed to these functions is the CVODES memory pointer returned by `CVodeCreate`; the second argument passed to these functions is the desired SUNLINSOL object to use for solving Newton systems. A call to one of these functions initializes the appropriate CVODES linear solver interface, linking this to the main CVODES 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 8 and 9.

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

#### `CVDlsSetLinearSolver`

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

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

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

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

`LS`            (SUNLinearSolver) SUNLINSOL object to use for solving Newton linear systems.

`J`             (SUNMatrix) SUNMATRIX object for used as a template for the Jacobian (must have a type compatible with the linear solver object).



|              |   |
|--------------|---|
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CVDLS_SUCCESS</code> The CVDLS initialization was successful.<br><code>CVDLS_MEM_NULL</code> The <code>ccode_mem</code> pointer is NULL.<br><code>CVDLS_ILL_INPUT</code> The CVDLS solver is not compatible with the LS or J input objects or is incompatible with the current NVECTOR module.<br><code>CVDLS_MEM_FAIL</code> A memory allocation request failed. |
| Notes        | 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 theaded NVECTOR module. Additional compatibility limitations for each SUNLINSOL object (i.e. SUNMATRIX and NVECTOR object compatibility) are described in Chapter 9.  |

#### CVSpilsSetLinearSolver

|              |  |
|--------------|--|
| Call         | <code>flag = CVSpilsSetLinearSolver(ccode_mem, LS);</code>   |
| Description  | The function <code>CVSpilsSetLinearSolver</code> attaches an iterative SUNLINSOL object <code>LS</code> to <code>CVODES</code> , initializing the CVSPILS scaled, preconditioned, iterative linear solver interface. The user's main program must include the <code>cvodes_spils.h</code> header file.   |
| Arguments    | <code>ccode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>LS</code> ( <code>SUNLinearSolver</code> ) SUNLINSOL object to use for solving Newton linear systems.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CVSPILS_SUCCESS</code> The CVSPILS initialization was successful.<br><code>CVSPILS_MEM_NULL</code> The <code>ccode_mem</code> pointer is NULL.<br><code>CVSPILS_ILL_INPUT</code> The CVSPILS solver is not compatible with the LS object or is incompatible with the current NVECTOR module.<br><code>CVSPILS_MEM_FAIL</code> A memory allocation request failed.<br><code>CVSPILS_SUNLS_FAIL</code> 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 <i>iterative</i> SUNLINSOL object. Additional compatibility limitations for each SUNLINSOL object (i.e. required NVECTOR routines) are described in Chapter 9.   |

#### CVDiag

|              |  |
|--------------|--|
| Call         | <code>flag = CVDiag(ccode_mem);</code>   |
| Description  | The function <code>CVDiag</code> selects the CVDIAG linear solver. The user's main program must include the <code>cvodes_diag.h</code> header file.  |
| Arguments    | <code>ccode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CVDIAG_SUCCESS</code> The CVDIAG initialization was successful.<br><code>CVDIAG_MEM_NULL</code> The <code>ccode_mem</code> pointer is NULL.<br><code>CVDIAG_ILL_INPUT</code> The CVDIAG solver is not compatible with the current NVECTOR module.<br><code>CVDIAG_MEM_FAIL</code> A memory allocation request failed. |
| Notes        | The CVDIAG solver is the simplest of all of the current CVODES linear solver interfaces. The CVDIAG solver uses an approximate diagonal Jacobian formed by way of a difference quotient. The user does <i>not</i> have the option of supplying a function to compute an approximate diagonal Jacobian.   |

#### 4.5.4 Rootfinding initialization function

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

|                      |   |
|----------------------|---|
| <b>CVodeRootInit</b> |   |
| Call                 | <code>flag = CVodeRootInit(cvode_mem, nrtfn, g);</code>   |
| Description          | The function <code>CVodeRootInit</code> specifies that the roots of a set of functions $g_i(t, y)$ are to be found while the IVP is being solved.   |
| Arguments            | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>nrtfn</code> (int) is the number of root functions <math>g_i</math>.</p> <p><code>g</code> (CVRootFn) is the C function which defines the <code>nrtfn</code> functions <math>g_i(t, y)</math> whose roots are sought. See §4.6.4 for details.</p>  |
| Return value         | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeRootInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The <code>cvode_mem</code> argument was <code>NULL</code>.</p> <p><code>CV_MEM_FAIL</code> A memory allocation failed.</p> <p><code>CV_ILL_INPUT</code> The function <code>g</code> is <code>NULL</code>, but <code>nrtfn &gt; 0</code>.</p> |
| Notes                | If a new IVP is to be solved with a call to <code>CVodeReInit</code> , where the new IVP has no rootfinding problem but the prior one did, then call <code>CVodeRootInit</code> with <code>nrtfn=0</code> .   |

#### 4.5.5 CVODES solver function

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

|              |  |
|--------------|--|
| <b>CVode</b> |  |
| Call         | <code>flag = CVode(cvode_mem, tout, yout, &amp;tret, itask);</code>  |
| Description  | The function <code>CVode</code> integrates the ODE over an interval in $t$ .   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>tout</code> (realtype) the next time at which a computed solution is desired.</p> <p><code>yout</code> (N_Vector) the computed solution vector.</p> <p><code>tret</code> (realtype) the time reached by the solver (output).</p> <p><code>itask</code> (int) a flag indicating the job of the solver for the next user step. The <code>CV_NORMAL</code> option causes the solver to take internal steps until it has reached or just passed the user-specified <code>tout</code> parameter. The solver then interpolates in order to return an approximate value of <math>y(\text{tout})</math>. The <code>CV_ONE_STEP</code> option tells the solver to take just one internal step and then return the solution at the point reached by that step.</p> |
| Return value | <p><code>CVode</code> returns a vector <code>yout</code> and a corresponding independent variable value <math>t = \text{tret}</math>, such that <code>yout</code> is the computed value of <math>y(t)</math>.</p> <p>In <code>CV_NORMAL</code> mode (with no errors), <code>tret</code> will be equal to <code>tout</code> and <code>yout = y(tout)</code>.</p> <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> <code>CVode</code> succeeded and no roots were found.</p>  |

|                       |   |
|-----------------------|---|
| CV_TSTOP_RETURN       | CVode succeeded by reaching the stopping point specified through the optional input function <code>CVodeSetStopTime</code> (see §4.5.6.1).  |
| CV_ROOT_RETURN        | CVode 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.   |
| CV_MEM_NULL           | The <code>cvode_mem</code> argument was NULL.   |
| CV_NO_MALLOC          | The CVODES memory was not allocated by a call to <code>CVodeInit</code> .   |
| CV_ILL_INPUT          | 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. |
| CV_TOO_CLOSE          | 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.  |
| CV_TOO_MUCH_WORK      | The solver took <code>mxstep</code> internal steps but still could not reach <code>tout</code> . The default value for <code>mxstep</code> is <code>MXSTEP_DEFAULT = 500</code> .   |
| CV_TOO_MUCH_ACC       | The solver could not satisfy the accuracy demanded by the user for some internal step.  |
| CV_ERR_FAILURE        | Either error test failures occurred too many times ( <code>MXNEF = 7</code> ) during one internal time step, or with $ h  = h_{min}$ .  |
| CV_CONV_FAILURE       | Either convergence test failures occurred too many times ( <code>MXNCF = 10</code> ) during one internal time step, or with $ h  = h_{min}$ .   |
| CV_LINIT_FAIL         | The linear solver's initialization function failed.   |
| CV_LSETUP_FAIL        | The linear solver's setup function failed in an unrecoverable manner.   |
| CV_LSOLVE_FAIL        | The linear solver's solve function failed in an unrecoverable manner.   |
| CV_RHSFUNC_FAIL       | The right-hand side function failed in an unrecoverable manner.   |
| CV_FIRST_RHSFUNC_FAIL | The right-hand side function had a recoverable error at the first call.   |
| CV_REPTD_RHSFUNC_ERR  | Convergence test failures occurred too many times due to repeated recoverable errors in the right-hand side function. This flag will also be returned if the right-hand side function had repeated recoverable errors during the estimation of an initial step size.  |
| CV_UNREC_RHSFUNC_ERR  | The right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the right-hand side function fails recoverably after an error test failed while at order one.   |
| CV_RTFUNC_FAIL        | The rootfinding function failed.  |

## Notes

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

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

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.

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

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

### 4.5.6 Optional input functions

There are numerous optional input parameters that control the behavior of the CVODES solver. CVODES provides functions that can be used to change these optional input parameters from their default values. Table 4.2 lists all optional input functions in CVODES which are then described in detail in the remainder of this section, beginning with those for the main CVODES solver and continuing with those for the linear solver interfaces. Note that the diagonal linear solver module has no optional inputs. For the most casual use of CVODES, the reader can skip to §4.6.

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

#### 4.5.6.1 Main solver optional input functions

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

##### `CVodeSetErrFile`

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

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

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

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

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

**CV\_SUCCESS** The optional value has been successfully set.

**CV\_MEM\_NULL** The **ccode\_mem** pointer is NULL.

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

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

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



#### **CVodeSetErrHandlerFn**

Call **flag = CVodeSetErrHandlerFn(ccode\_mem, ehfun, eh\_data);**

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

Arguments **ccode\_mem** (void \*) pointer to the CVOIDES memory block.

**ehfun** (CVerHandlerFn) is the C error handler function (see §4.6.2).

**eh\_data** (void \*) pointer to user data passed to **ehfun** every time it is called.

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

**CV\_SUCCESS** The function **ehfun** and data pointer **eh\_data** have been successfully set.

**CV\_MEM\_NULL** The **ccode\_mem** pointer is NULL.

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

#### **CVodeSetUserData**

Call **flag = CVodeSetUserData(ccode\_mem, user\_data);**

Description The function **CVodeSetUserData** specifies the user data block **user\_data** and attaches it to the main CVOIDES memory block.

Arguments **ccode\_mem** (void \*) pointer to the CVOIDES memory block.

**user\_data** (void \*) pointer to the user data.

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

**CV\_SUCCESS** The optional value has been successfully set.

**CV\_MEM\_NULL** The **ccode\_mem** pointer is NULL.

Notes If specified, the pointer to **user\_data** is passed to all user-supplied functions that have it as an argument. Otherwise, a NULL pointer is passed.

If **user\_data** is needed in user linear solver or preconditioner functions, the call to **CVodeSetUserData** must be made *before* the call to specify the linear solver.



#### **CVodeSetMaxOrd**

Call **flag = CVodeSetMaxOrder(ccode\_mem, maxord);**

Description The function **CVodeSetMaxOrder** specifies the maximum order of the linear multistep method.

Arguments **ccode\_mem** (void \*) pointer to the CVOIDES 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 CVODES memory block, its value cannot be increased past its previous value.

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

#### CVodeSetMaxNumSteps

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

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

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

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

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

Notes Passing `mxsteps = 0` results in CVODES using the default value (500).  
 Passing `mxsteps < 0` disables the test (*not recommended*).

#### CVodeSetMaxHnilWarns

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

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

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

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

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

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

#### CVodeSetStabLimDet

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

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`stldet` (`booleantype`) flag controlling stability limit detection (`SUNTRUE = on`; `SUNFALSE = off`).

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

- `CV_SUCCESS` The optional value has been successfully set.
- `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.
- `CV_ILL_INPUT` The linear multistep method is not set to `CV_BDF`.

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

#### CVodeSetInitStep

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

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`hin` (`realtype`) value of the initial step size to be attempted. Pass 0.0 to use the default value.

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

`CV_SUCCESS` The optional value has been successfully set.

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

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

#### CVodeSetMinStep

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

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`hmin` (`realtype`) minimum absolute value of the step size ( $\geq 0.0$ ).

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 CVODES 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 `cvode_mem` pointer is `NULL`.

`CV_ILL_INPUT` Either `hmax` is nonpositive or it is smaller than the minimum allowable step size.

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

**CVodeSetStopTime**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSetStopTime(cvode_mem, tstop);</code>   |
| Description  | The function <code>CVodeSetStopTime</code> specifies the value of the independent variable $t$ past which the solution is not to proceed.   |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>tstop</code> (realtype) value of the independent variable past which the solution should not proceed.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.<br><code>CV_ILL_INPUT</code> The value of <code>tstop</code> 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.  |

**CVodeSetMaxErrTestFails**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSetMaxErrTestFails(cvode_mem, maxnef);</code>   |
| Description  | The function <code>CVodeSetMaxErrTestFails</code> specifies the maximum number of error test failures permitted in attempting one step.   |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>maxnef</code> (int) maximum number of error test failures allowed on one step ( $> 0$ ).   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. |
| Notes        | The default value is 7.   |

**CVodeSetMaxNonlinIters**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSetMaxNonlinIters(cvode_mem, maxcor);</code>  |
| Description  | The function <code>CVodeSetMaxNonlinIters</code> specifies the maximum number of nonlinear solver iterations permitted per step.  |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>maxcor</code> (int) maximum number of nonlinear solver iterations allowed per step ( $> 0$ ).  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer 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> (void *) pointer to the CVODES memory block.<br><code>maxncf</code> (int) 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<br><code>CV_SUCCESS</code> The optional value has been successfully set.                                      |



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

Notes The default value is 10.

#### CVodeSetNonlinConvCoef

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

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

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

Return value The return value `flag` (of type `int`) is one of  
 CV\_SUCCESS The optional value has been successfully set.  
 CV\_MEM\_NULL The `cvode_mem` pointer is NULL.

Notes The default value is 0.1.

#### CVodeSetIterType

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

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

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

Return value The return value `flag` (of type `int`) is one of  
 CV\_SUCCESS The optional value has been successfully set.  
 CV\_MEM\_NULL The `cvode_mem` pointer is NULL.  
 CV\_ILL\_INPUT The `iter` value passed is neither `CV_NEWTON` nor `CV_FUNCTIONAL`.

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

#### 4.5.6.2 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 `flag = CVDlsSetJacFn(cvode_mem, jac);`

Description The function `CVDlsSetJacFn` specifies the Jacobian approximation function to be used.

Arguments `cvode_mem` (void \*) pointer to the CVODES memory block.  
`jac` (CVDlsJacFn) user-defined Jacobian approximation function.

Return value The return value `flag` (of type `int`) is one of  
 CVDLS\_SUCCESS 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 <code>CVDLS</code> linear solver interface has not been initialized.  |
| Notes | By default, <code>CVDLS</code> 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.  |

#### 4.5.6.3 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 <code>CVODES</code> memory block.<br><code>psetup</code> ( <code>CVSpilsPrecSetupFn</code> ) user-defined preconditioner setup function. Pass <code>NULL</code> if no setup is necessary.<br><code>psolve</code> ( <code>CVSpilsPrecSolveFn</code> ) user-defined preconditioner solve function.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CVSPILS_SUCCESS</code> The optional values have been successfully set.<br><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CVSPILS_LMEM_NULL</code> The <code>CVSPILS</code> linear solver has not been initialized.<br><code>CVSPILS_SUNLS_FAIL</code> An error occurred when setting up preconditioning in the <code>SUNLINSOL</code> object used by the <code>CVSPILS</code> 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, jtimes);</code>   |
| Description  | The function <code>CVSpilsSetJacTimes</code> specifies the Jacobian-vector setup and product functions.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>jtsetup</code> (CVSpilsJacTimesSetupFn) user-defined Jacobian-vector setup function. Pass NULL if no setup is necessary.</p> <p><code>jtimes</code> (CVSpilsJacTimesVecFn) user-defined Jacobian-vector product function.</p>   |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVSPILS_SUCCESS</code> The optional value has been successfully set.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</p> <p><code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.</p> <p><code>CVSPILS_SUNLS_FAIL</code> An error occurred when setting up the system matrix-times-vector routines in the SUNLINSOL object used by the CVSPILS interface.</p> |
| Notes        | <p>By default, the CVSPILS linear solvers use an internal difference quotient function. If NULL is passed to <code>jtimes</code>, this default function is used.</p> <p>The function type <code>CVSpilsJacTimesSetupFn</code> is described in §4.6.7.</p> <p>The function type <code>CVSpilsJacTimesVecFn</code> is described in §4.6.6.</p>  |

**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 Newton iteration test constant.  |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>eplifac</code> (realtype) linear convergence safety factor (<math>\geq 0.0</math>).</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVSPILS_SUCCESS</code> The optional value has been successfully set.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</p> <p><code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.</p> <p><code>CVSPILS_ILL_INPUT</code> The factor <code>eplifac</code> is negative.</p> |
| Notes        | <p>The default value is 0.05.</p> <p>If <code>eplifac</code>= 0.0 is passed, the default value is used.</p>  |

**4.5.6.4 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   | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>rootdir</code> (int *) state array of length <code>nrtfn</code>, the number of root functions <math>g_i</math>, 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 <math>g_i</math> should be reported. A value of +1 or -1 indicates that the solver should report only zero-crossings where <math>g_i</math> is increasing or decreasing, respectively.</p> |

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

- CV\_SUCCESS** The optional value has been successfully set.
- CV\_MEM\_NULL** The **cvode\_mem** pointer is **NULL**.
- CV\_ILL\_INPUT** rootfinding has not been activated through a call to **CVodeRootInit**.

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

#### CVodeSetNoInactiveRootWarn

Call **flag = CVodeSetNoInactiveRootWarn(cvode\_mem);**

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

Arguments **cvode\_mem** (**void \***) pointer to the CVODES memory block.

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

- CV\_SUCCESS** The optional value has been successfully set.
- CV\_MEM\_NULL** The **cvode\_mem** pointer is **NULL**.

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

### 4.5.7 Interpolated output function

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

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

#### CVodeGetDky

Call **flag = CVodeGetDky(cvode\_mem, t, k, dky);**

Description The function **CVodeGetDky** computes the  $k$ -th derivative of the function  $y$  at time  $t$ , i.e.  $d^{(k)}y/dt^{(k)}(t)$ , where  $t_n - h_u \leq t \leq t_n$ ,  $t_n$  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 **qlast**).

Arguments **cvode\_mem** (**void \***) pointer to the CVODES memory block.

**t** (**realtype**) the value of the independent variable at which the derivative is to be evaluated.

**k** (**int**) the derivative order requested.

**dky** (**N\_Vector**) vector containing the derivative. This vector must be allocated by the user.

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

- CV\_SUCCESS** **CVodeGetDky** succeeded.
- CV\_BAD\_K**  $k$  is not in the range  $0, 1, \dots, q_u$ .
- CV\_BAD\_T**  $t$  is not in the interval  $[t_n - h_u, t_n]$ .
- CV\_BAD\_DKY** The **dky** argument was **NULL**.
- CV\_MEM\_NULL** The **cvode\_mem** argument was **NULL**.

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

### 4.5.8 Optional output functions

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

Some of the optional outputs, especially the various counters, can be very useful in determining how successful the CVODES solver is in doing its job. For example, the counters `nsteps` and `nfevals` provide a rough measure of the overall cost of a given run, and can be compared among runs with differing input options to suggest which set of options is most efficient. The ratio `nniters/nsteps` measures the performance of the Newton iteration 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.

#### 4.5.8.1 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.<br><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.<br><code>minor</code> ( <code>int</code> ) SUNDIALS release minor version number.<br><code>patch</code> ( <code>int</code> ) SUNDIALS release patch version number.<br><code>label</code> ( <code>char *</code> ) character array to hold the SUNDIALS release label.<br><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 CVODES, CVDLS, CVDIAG, and CVSPILS

| Optional output   | Function name                  |
|---|--------------------------------|
| <b>CVODES main solver</b>                                   |                                |
| Size of CVODES real and integer workspaces                  | CVodeGetWorkSpace              |
| Cumulative number of internal steps                         | CVodeGetNumSteps               |
| No. of calls to r.h.s. function                             | CVodeGetNumRhsEvals            |
| No. of calls to linear solver setup function                | CVodeGetNumLinSolvSetups       |
| No. of local error test failures that have occurred         | CVodeGetNumErrTestFails        |
| Order used during the last step                             | CVodeGetLastOrder              |
| Order to be attempted on the next step                      | CVodeGetCurrentOrder           |
| No. of order reductions due to stability limit detection    | CVodeGetNumStabLimOrderReds    |
| Actual initial step size used                               | CVodeGetActualInitStep         |
| Step size used for the last step                            | CVodeGetLastStep               |
| Step size to be attempted on the next step                  | CVodeGetCurrentStep            |
| Current internal time reached by the solver                 | CVodeGetCurrentTime            |
| Suggested factor for tolerance scaling                      | CVodeGetTolScaleFactor         |
| Error weight vector for state variables                     | CVodeGetErrWeights             |
| Estimated local error vector                                | CVodeGetEstLocalErrors         |
| No. of nonlinear solver iterations                          | CVodeGetNumNonlinSolvIters     |
| No. of nonlinear convergence failures                       | CVodeGetNumNonlinSolvConvFails |
| All CVODES integrator statistics                            | CVodeGetIntegratorStats        |
| CVODES nonlinear solver statistics                          | CVodeGetNonlinSolvStats        |
| Array showing roots found                                   | CVodeGetRootInfo               |
| No. of calls to user root function                          | CVodeGetNumGEvals              |
| Name of constant associated with a return flag              | CVodeGetReturnFlagName         |
| <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       |

## 4.5.8.2 Main solver optional output functions

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

**CVodeGetWorkSpace**

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

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

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

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

Notes In terms of the problem size  $N$ , the maximum method order `maxord`, and the number `nrtfn` of root functions (see §4.5.4), 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  $\text{leniw} = 50$

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

**CVodeGetNumSteps**

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

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

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is NULL.

#### CVodeGetNumRhsEvals

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

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

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is NULL.

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

#### CVodeGetNumLinSolvSetups

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

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

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nlinsetups` (`long int`) number of calls made to the linear solver setup function.

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is NULL.

#### CVodeGetNumErrTestFails

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

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

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is NULL.

#### CVodeGetLastOrder

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

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

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

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

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

`CV_MEM_NULL` The `cvode_mem` pointer is NULL.



**CVodeGetCurrentOrder**

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

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

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

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

**CVodeGetLastStep**

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

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

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

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

**CVodeGetCurrentStep**

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

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

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`hcur` (`realtype`) step size to be attempted on the next internal step.

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

**CVodeGetActualInitStep**

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

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

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

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

**Notes** Even if the value of the initial integration step size was specified by the user through a call to `CVodeSetInitStep`, this value might have been changed by CVODES to ensure that the step size is within the prescribed bounds ( $h_{\min} \leq h_0 \leq h_{\max}$ ), 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 CVODES 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 CVODES 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 CVODES memory block.  
`tolsfac` (`realtype`) suggested scaling factor for user-supplied tolerances.

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

**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 CVODES memory block.  
`eweight` (`N_Vector`) solution error weights at the current time.

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

**Notes** The user must allocate memory for `eweight`.



## CNodeGetEstLocalErrors

Call `flag = CNodeGetEstLocalErrors(cvode_mem, ele):`

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

|           |   |
|-----------|---|
| Arguments | <code>cvoid_mem</code> (void *) pointer to the CVODES memory block. |
|           | <code>ele</code> (N_Vector) estimated local errors.                 |

|              |  |
|--------------|--|
| 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>cnode_mem</code> pointer is <code>NULL</code> . |

|       |  |
|-------|--|
| Notes | The user must allocate memory for <code>ele</code> . |
|-------|--|

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

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



## CNodeGetIntegratorStats

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

|             |  |
|-------------|--|
| Description | The function <code>CVodeGetIntegratorStats</code> returns the CVODES integrator statistics as a group. |
|-------------|--|

|           |                         |   |
|-----------|-------------------------|---|
| Arguments | <code>cvoid_mem</code>  | ( <code>void *</code> ) pointer to the CVOIDS memory block.                         |
|           | <code>nsteps</code>     | ( <code>long int</code> ) number of steps taken by CVOIDS.                          |
|           | <code>nfevals</code>    | ( <code>long int</code> ) number of calls to the user's <code>f</code> function.    |
|           | <code>nlinsetups</code> | ( <code>long int</code> ) number of calls made to the linear solver setup function. |
|           | <code>netfails</code>   | ( <code>long int</code> ) number of error test failures.                            |
|           | <code>qlast</code>      | ( <code>int</code> ) method order used on the last internal step.                   |
|           | <code>qcur</code>       | ( <code>int</code> ) method order to be used on the next internal step.             |
|           | <code>hinused</code>    | ( <code>realtype</code> ) actual value of initial step size.                        |
|           | <code>hlast</code>      | ( <code>realtype</code> ) step size taken on the last internal step.                |
|           | <code>hcur</code>       | ( <code>realtype</code> ) step size to be attempted on the next internal step.      |
|           | <code>tcur</code>       | ( <code>realtype</code> ) current internal time reached.                            |

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

- CV\_SUCCESS** the optional output values have been successfully set.
- CV\_MEM\_NULL** the **cnode\_mem** pointer is **NULL**.

CVodeGetNumNonlinSolvIters

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

|             |   |
|-------------|---|
| Description | The function <code>CVodeGetNumNonlinSolvIters</code> returns the number of nonlinear (functional or Newton) iterations performed. |
|-------------|---|

|           |                        |  |
|-----------|------------------------|--|
| Arguments | <code>cvoid_mem</code> | (void *) pointer to the CVODES memory block.         |
|           | <code>nniters</code>   | (long int) number of nonlinear iterations performed. |

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

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

#### CVodeGetNumNonlinSolvConvFails

**Call** `flag = CVodeGetNumNonlinSolvConvFails(cvode_mem, &nncfails);`  
**Description** The function `CVodeGetNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nncfails` (`long int`) number of nonlinear convergence failures.  
**Return value** The return value `flag` (of type `int`) is one of  
 CV\_SUCCESS The optional output value has been successfully set.  
 CV\_MEM\_NULL The `cvode_mem` pointer is NULL.

#### CVodeGetNonlinSolvStats

**Call** `flag = CVodeGetNonlinSolvStats(cvode_mem, &nniters, &nncfails);`  
**Description** The function `CVodeGetNonlinSolvStats` returns the CVODES nonlinear solver statistics as a group.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nniters` (`long int`) number of nonlinear iterations performed.  
`nncfails` (`long int`) number of nonlinear convergence failures.  
**Return value** The return value `flag` (of type `int`) is one of  
 CV\_SUCCESS The optional output value has been successfully set.  
 CV\_MEM\_NULL The `cvode_mem` pointer is NULL.

#### CVodeGetReturnFlagName

**Call** `name = CVodeGetReturnFlagName(flag);`  
**Description** The function `CVodeGetReturnFlagName` returns the name of the CVODES constant corresponding to `flag`.  
**Arguments** The only argument, of type `int`, is a return flag from a CVODES function.  
**Return value** The return value is a string containing the name of the corresponding constant.

### 4.5.8.3 Rootfinding optional output functions

There are two optional output functions associated with rootfinding.

#### CVodeGetRootInfo

**Call** `flag = CVodeGetRootInfo(cvode_mem, rootsfound);`  
**Description** The function `CVodeGetRootInfo` returns an array showing which functions were found to have a root.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`rootsfound` (`int *`) array of length `nrtfn` with the indices of the user functions  $g_i$  found to have a root. For  $i = 0, \dots, \text{nrtfn}-1$ , `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 CVODES memory block.  
`ngevals` (long int) number of calls made to the user's function  $g$  thus far.
- Return value The return value `flag` (of type `int`) is one of:  
**CV\_SUCCESS** The optional output value has been successfully set.  
**CV\_MEM\_NULL** The `cvode_mem` pointer is NULL.

#### 4.5.8.4 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 CVODES 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 CVODES memory block.  
`njevals` (long int) the number of calls to the Jacobian function.
- Return value The return value `flag` (of type `int`) is one of

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

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

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 CVODES 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".

#### 4.5.8.5 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 CVODES memory block.<br><code>lenrwLS</code> (long int) the number of <code>realtype</code> values in the CVSPILS workspace.<br><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<br><code>CVSPILS.SUCCESS</code> The optional output value has been successfully set.<br><code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.<br><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.<br>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 CVODES memory block.<br><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<br><code>CVSPILS.SUCCESS</code> The optional output value has been successfully set.<br><code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.<br><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 CVODES memory block.<br><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<br><code>CVSPILS.SUCCESS</code> The optional output value has been successfully set.<br><code>CVSPILS.MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.<br><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 CVODES memory block.  
                  `npevals` (long int) the current number of calls to `psetup`.

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

`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 CVODES memory block.  
                  `npsolves` (long int) the current number of calls to `psolve`.

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

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

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

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

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

`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> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nfevalsLS</code> ( <code>long int</code> ) 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<br><code>CVSPILS_SUCCESS</code> The optional output value has been successfully set.<br><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><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> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>lsflag</code> ( <code>long int</code> ) the value of the last return flag from a CVSPILS function.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of<br><code>CVSPILS_SUCCESS</code> The optional output value has been successfully set.<br><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><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> .<br>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 <code>SUNLINSOL</code> object, which will be one of: <code>SUNLS_MEM_NULL</code> , indicating that the <code>SUNLINSOL</code> memory is <code>NULL</code> ; <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 <code>long int</code> , is a return flag from a CVSPILS function.                                       |
| Return value | The return value is a string containing the name of the corresponding constant.  |

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

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

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

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

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

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

**CVDiagGetNumRhsEvals**

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

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

**Arguments**    `cvode_mem` (void \*) pointer to the CVODES memory block.  
                  `nfevalsLS` (long int) the number of calls made to the user-supplied right-hand side function.

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

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

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

**CVDiagGetLastFlag**

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

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

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

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

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

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

**CVDiagGetReturnFlagName**

|              |  |
|--------------|--|
| 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.  |

**4.5.9 CVODES reinitialization function**

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

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

If there are changes to the linear solver specifications, make the appropriate calls to either the linear solver objects themselves, or to the 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 extension over the discontinuity, so that the step across it (and subsequent rootfinding, if used) can be done efficiently. Then use a switch within the RHS function (communicated through `user_data`) that can be flipped between the stopping of the integration and the restart, so that the restarted problem uses the new values (which have jumped). Similar comments apply if there is to be a jump in the dependent variable vector.

**CVodeReInit**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeReInit(cvode_mem, t0, y0);</code>  |
| Description  | The function <code>CVodeReInit</code> provides required problem specifications and reinitializes CVODES.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>t0</code> ( <code>realtype</code> ) is the initial value of $t$ .<br><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: <ul style="list-style-type: none"> <li><code>CV_SUCCESS</code> The call to <code>CVodeReInit</code> was successful.</li> <li><code>CV_MEM_NULL</code> The CVODES memory block was not initialized through a previous call to <code>CVodeCreate</code>.</li> <li><code>CV_NO_MALLOC</code> Memory space for the CVODES memory block was not allocated through a previous call to <code>CVodeInit</code>.</li> <li><code>CV_ILL_INPUT</code> An input argument to <code>CVodeReInit</code> has an illegal value.</li> </ul> |
| 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 (if Newton iteration is chosen), 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:

|              |  |
|--------------|--|
|              | <div style="border: 1px solid black; padding: 2px; display: inline-block;"><code>CVRhsFn</code></div>  |
| 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><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the dependent variable vector, <math>y(t)</math>.</p> <p><code>ydot</code> is the output vector <math>f(t, y)</math>.</p> <p><code>user_data</code> is the <code>user_data</code> pointer passed to <code>CVodeSetUserData</code>.</p> |
| Return value | A <code>CVRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES 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        | Allocation of memory for <code>ydot</code> is handled within CVODES.   |

A recoverable failure error return from the `CVRhsFn` is typically used to flag a value of the dependent variable  $y$  that is “illegal” in some way (e.g., negative where only a non-negative value is physically meaningful). If such a return is made, CVODES will attempt to recover (possibly repeating the Newton iteration, or reducing the step size) in order to avoid this recoverable error return.

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

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



**CVRootFn**

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

**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   | <code>typedef (*CVDlsJacFn)(realtype t, N_Vector y, N_Vector fy,<br/>SUNMatrix Jac, void *user_data,<br/>N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);</code>  |
| Purpose      | This function computes the Jacobian matrix $J = \partial f / \partial y$ (or an approximation to it).  |
| Arguments    | <p><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the dependent variable vector, namely the predicted value of <math>y(t)</math>.</p> <p><code>fy</code> is the current value of the vector <math>f(t, y)</math>.</p> <p><code>Jac</code> is the output Jacobian matrix (of type <code>SUNMatrix</code>).</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> <p><code>tmp1</code><br/><code>tmp2</code><br/><code>tmp3</code> are pointers to memory allocated for variables of type <code>N_Vector</code> which can be used by a <code>CVDlsJacFn</code> function as temporary storage or work space.</p>           |
| Return value | A <code>CVDlsJacFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODES</code> will attempt to correct, while <code>CVDLS</code> sets <code>last_flag</code> to <code>CVDLS_JACFUNC_RECVR</code> ), or a negative value if it failed unrecoverably (in which case the integration is halted, <code>CVodes</code> returns <code>CV_LSETUP_FAIL</code> and <code>CVDLS</code> sets <code>last_flag</code> to <code>CVDLS_JACFUNC_UNRECVR</code> ).   |
| Notes        | <p>Information regarding the structure of the specific <code>SUNMATRIX</code> structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific <code>SUNMATRIX</code> interface functions (see Chapter 8 for details).</p> <p>Prior to calling the user-supplied Jacobian function, the Jacobian matrix <math>J(t, y)</math> is zeroed out, so only nonzero elements need to be loaded into <code>Jac</code>.</p> <p>If the user's <code>CVDlsJacFn</code> 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 <code>cv_mem</code></p> |

to `user_data` and then use the `CVodeGet*` functions described in §4.5.8.2. 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 §8.1.

#### **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 §8.2.

#### **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 §8.3.

#### 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    | <code>v</code>  | is the vector by which the Jacobian must be multiplied.   |  |
|              | <code>Jv</code>   | is the output vector computed.  |  |
|              | <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>user_data</code>  | is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> . |  |
|              | <code>tmp</code>  | is a pointer to memory allocated for a variable of type <code>N_Vector</code> 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        | If the user's <code>CVSpilsJacTimesVecFn</code> 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 <code>cv_mem</code> to <code>user_data</code> and then use the <code>CVodeGet*</code> functions described in §4.5.8.2. The unit roundoff can be accessed as <code>UNIT_ROUNDOFF</code> defined in <code>sundials_types.h</code> . |   |  |

#### 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:

`CVSpilsJacTimesSetupFn`

|              |  |   |  |
|--------------|--|---|--|
| Definition   | <pre>typedef int (*CVSpilsJacTimesSetupFn)(realtype t, N_Vector y,<br/>                                       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** Each call to the Jacobian-vector setup function is preceded by a call to the `CVRhsFn` user function with the same `(t,y)` arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.

If the user's `CVSpilsJacTimesSetupFn` function uses difference quotient approximations, it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.8.2. 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 Newton 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** `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);`

**Purpose** This function solves the preconditioned system  $Pz = r$ .

**Arguments**

- `t` is the current value of the independent variable.
- `y` is the current value of the dependent variable vector.
- `fy` is the current value of the vector  $f(t, y)$ .
- `r` is the right-hand side vector of the linear system.
- `z` is the computed output vector.
- `gamma` is the scalar  $\gamma$  appearing in the Newton matrix given by  $M = I - \gamma J$ .
- `delta` is an input tolerance to be used if an iterative method is employed in the solution. In that case, the residual vector  $Res = r - Pz$  of the system should be made less than `delta` in the weighted  $l_2$  norm, i.e.,  $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} < \text{delta}$ . To obtain the `N_Vector ewt`, call `CVodeGetErrWeights` (see §4.5.8.2).
- `lr` is an input flag indicating whether the preconditioner solve function is to use the left preconditioner (`lr = 1`) or the right preconditioner (`lr = 2`);
- `user_data` is a pointer to user data, the same as the `user_data` parameter passed to the function `CVodeSetUserData`.

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

#### 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** `typedef int (*CVSpilsPrecSetupFn)(realtype t, N_Vector y, N_Vector fy,  
booleantype jok, booleantype *jcurPtr,  
realtype gamma, void *user_data);`

|              |   |  |
|--------------|---|--|
| Purpose      | This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner.   |  |
| Arguments    | <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 $y(t)$ .  |
|              | <code>fy</code>   | is the current value of the vector $f(t, y)$ .   |
|              | <code>jok</code>  | is an input flag indicating whether the Jacobian-related data needs to be updated. The <code>jok</code> argument provides for the reuse of Jacobian data in the preconditioner solve function. <code>jok = SUNFALSE</code> means that the Jacobian-related data must be recomputed from scratch. <code>jok = SUNTRUE</code> means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of <code>gamma</code> ). A call with <code>jok = SUNTRUE</code> can only occur after a call with <code>jok = SUNFALSE</code> . |
|              | <code>jcurPtr</code>  | is a pointer to a flag which should be set to <code>SUNTRUE</code> if Jacobian data was recomputed, or set to <code>SUNFALSE</code> if Jacobian data was not recomputed, but saved data was still reused.  |
|              | <code>gamma</code>  | is the scalar $\gamma$ appearing in the Newton matrix $M = I - \gamma J$ .   |
|              | <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 setup function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).  |  |
| Notes        | The operations performed by this function might include forming a crude approximate Jacobian and performing an LU factorization of the resulting approximation to $M = I - \gamma J$ .  |  |
|              | Each call to the preconditioner setup function is preceded by a call to the <code>CVRhsFn</code> user function with the same <code>(t,y)</code> arguments. Thus, the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.  |  |
|              | This function is not called in advance of every call to the preconditioner solve function, but rather is called only as often as needed to achieve convergence in the Newton iteration.   |  |
|              | If the user's <code>CVSpilsPrecSetupFn</code> 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 <code>cv_mem</code> to <code>user_data</code> and then use the <code>CVodeGet*</code> functions described in §4.5.8.2. The unit roundoff can be accessed as <code>UNIT_ROUNDOFF</code> defined in <code>sundials_types.h</code> . |  |

## 4.7 Integration of pure quadrature equations

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

1. Initialize parallel or multi-threaded environment, if appropriate
2. Set problem dimensions, etc.

Set the problem size  $N$  (excluding quadrature variables), and the number of quadrature variables  $N_q$ .

If appropriate, set the local vector length  $N_{local}$  (excluding quadrature variables), and the local number of quadrature variables  $N_{qlocal}$ .

3. **Set vector of initial values**

4. **Create CVODES object**

5. **Allocate internal memory**

6. **Set optional inputs**

7. **Attach linear solver module**

8. **Set linear solver optional inputs**

9. **Set vector  $y_{Q0}$  of initial values for quadrature variables**

Typically, the quadrature variables should be initialized to 0.

10. **Initialize quadrature integration**

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

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

Call `CVodeSetQuadErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism, and to specify the integration tolerances for quadrature variables. See §4.7.4 for details.

12. **Advance solution in time**

13. **Extract quadrature variables**

Call `CVodeGetQuad` to obtain the values of the quadrature variables at the current time. See §4.7.3 for details.

14. **Get optional outputs**

15. **Get quadrature optional outputs**

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

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

17. **Free solver memory**

18. **Finalize MPI, if used**

`CVodeQuadInit` can be called and quadrature-related optional inputs (step 11 above) can be set anywhere between steps 4 and 12.

### 4.7.1 Quadrature initialization and deallocation functions

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

**CVodeQuadInit**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeQuadInit(cvode_mem, fQ, yQ0);</code>  |
| Description  | The function <code>CVodeQuadInit</code> provides required problem specifications, allocates internal memory, and initializes quadrature integration.  |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>fQ</code> (<code>CVQuadRhsFn</code>) is the C function which computes <math>f_Q</math>, the right-hand side of the quadrature equations. This function has the form <code>fQ(t, y, yQdot, fQ_data)</code> (for full details see §4.7.6).</p> <p><code>yQ0</code> (<code>N_Vector</code>) is the initial value of <code>yQ</code>.</p> |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <p><code>CV_SUCCESS</code> The call to <code>CVodeQuadInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODES memory was not initialized by a prior call to <code>CVodeCreate</code>.</p> <p><code>CV_MEM_FAIL</code> A memory allocation request failed.</p>   |
| Notes        | If an error occurred, <code>CVodeQuadInit</code> also sends an error message to the error handler function.   |

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

- Base value:  $\text{lenrw} = \text{lenrw} + (\text{maxord}+5)N_q$
- If using `CVodeSVtolerances` (see `CVodeSetQuadErrCon`):  $\text{lenrw} = \text{lenrw} + N_q$

the size of the integer workspace is increased as follows:

- Base value:  $\text{leniw} = \text{leniw} + (\text{maxord}+5)N_q$
- If using `CVodeSVtolerances`:  $\text{leniw} = \text{leniw} + N_q$

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

**CVodeQuadReInit**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeQuadReInit(cvode_mem, yQ0);</code>  |
| Description  | The function <code>CVodeQuadReInit</code> provides required problem specifications and reinitializes the quadrature integration.  |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block.</p> <p><code>yQ0</code> (<code>N_Vector</code>) is the initial value of <code>yQ</code>.</p>  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <p><code>CV_SUCCESS</code> The call to <code>CVodeReInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODES memory was not initialized by a prior call to <code>CVodeCreate</code>.</p> <p><code>CV_NO_QUAD</code> Memory space for the quadrature integration was not allocated by a prior call to <code>CVodeQuadInit</code>.</p> |
| Notes        | If an error occurred, <code>CVodeQuadReInit</code> also sends an error message to the error handler function.   |

**CVodeQuadFree**

Call `CVodeQuadFree(cvode_mem);`

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

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

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

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

**4.7.2 CVODES solver function**

Even if quadrature integration was enabled, the call to the main solver function `CVode` is exactly the same as in §4.5.5. However, in this case the return value `flag` can also be one of the following:

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

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

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

`CV_UNREC_RHSFUNC_ERR` The quadrature right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the quadrature right-hand side function fails recoverably after an error test failed while at order one.

**4.7.3 Quadrature extraction functions**

If quadrature integration has been initialized by a call to `CVodeQuadInit`, or reinitialized by a call to `CVodeQuadReInit`, then CVODES computes both a solution and quadratures at time `t`. However, `CVode` will still return only the solution  $y$  in `yout`. Solution quadratures can be obtained using the following function:

**CVodeGetQuad**

Call `flag = CVodeGetQuad(cvode_mem, &tret, yQ);`

Description The function `CVodeGetQuad` returns the quadrature solution vector after a successful return from `CVode`.

Arguments `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.

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

`yQ` (`N_Vector`) the computed quadrature vector.

Return value The return value `flag` of `CVodeGetQuad` is one of:

`CV_SUCCESS` `CVodeGetQuad` was successful.

`CV_MEM_NULL` `cvode_mem` was `NULL`.

`CV_NO_QUAD` Quadrature integration was not initialized.

`CV_BAD_DKY` `yQ` is `NULL`.

Notes In case of an error return, an error message is also sent to the error handler function.

The function `CVodeGetQuadDky` computes the  $k$ -th derivatives of the interpolating polynomials for the quadrature variables at time `t`. This function is called by `CVodeGetQuad` with  $k = 0$  and with the current time at which `CVode` has returned, but may also be called directly by the user.

**CVodeGetQuadDky**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetQuadDky(cvode_mem, t, k, dkyQ);</code>  |
| Description  | The function <code>CVodeGetQuadDky</code> returns derivatives of the quadrature solution vector after a successful return from <code>CVode</code> .  |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the memory previously allocated by <code>CVodeInit</code>.</p> <p><code>t</code> (<code>realtype</code>) the time at which quadrature information is requested. The time <code>t</code> must fall within the interval defined by the last successful step taken by CVODES.</p> <p><code>k</code> (<code>int</code>) order of the requested derivative. This must be <math>\leq</math> <code>qlast</code>.</p> <p><code>dkyQ</code> (<code>N_Vector</code>) the vector containing the derivative. This vector must be allocated by the user.</p> |
| Return value | <p>The return value <code>flag</code> of <code>CVodeGetQuadDky</code> is one of:</p> <p><code>CV_SUCCESS</code> <code>CVodeGetQuadDky</code> succeeded.</p> <p><code>CV_MEM_NULL</code> The pointer to <code>cvode_mem</code> was NULL.</p> <p><code>CV_NO_QUAD</code> Quadrature integration was not initialized.</p> <p><code>CV_BAD_DKY</code> The vector <code>dkyQ</code> is NULL.</p> <p><code>CV_BAD_K</code> <code>k</code> is not in the range <math>0, 1, \dots, \text{qlast}</math>.</p> <p><code>CV_BAD_T</code> The time <code>t</code> is not in the allowed range.</p>                      |
| Notes        | In case of an error return, an error message is also sent to the error handler function.   |

#### 4.7.4 Optional inputs for quadrature integration

CVODES provides the following optional input functions to control the integration of quadrature equations.

**CVodeSetQuadErrCon**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeSetQuadErrCon(cvode_mem, errconQ);</code>  |
| Description  | The function <code>CVodeSetQuadErrCon</code> specifies whether or not the quadrature variables are to be used in the step size control mechanism within CVODES. If they are, the user must call <code>CVodeQuadSStolerances</code> or <code>CVodeQuadSVtolerances</code> to specify the integration tolerances for the quadrature variables. |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block.</p> <p><code>errconQ</code> (<code>booleantype</code>) specifies whether quadrature variables are included (<code>SUNTRUE</code>) or not (<code>SUNFALSE</code>) in the error control mechanism.</p>   |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CV_SUCCESS</code> The optional value has been successfully set.</p> <p><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</p> <p><code>CV_NO_QUAD</code> Quadrature integration has not been initialized.</p>                     |
| Notes        | <p>By default, <code>errconQ</code> is set to <code>SUNFALSE</code>.</p> <p>It is illegal to call <code>CVodeSetQuadErrCon</code> before a call to <code>CVodeQuadInit</code>.</p>   |



If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

**CVodeQuadSStolerances**

|             |  |
|-------------|--|
| Call        | <code>flag = CVodeQuadSVtolerances(cvode_mem, reltolQ, abstolQ);</code>                            |
| Description | The function <code>CVodeQuadSStolerances</code> specifies scalar relative and absolute tolerances. |
| Arguments   | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.                 |

`reltolQ` (`realtype`) is the scalar relative error tolerance.  
`abstolQ` (`realtype`) is the scalar absolute error tolerance.

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

`CV_SUCCESS` The optional value has been successfully set.  
`CV_NO_QUAD` Quadrature integration was not initialized.  
`CV_MEM_NULL` The `cnode_mem` pointer is `NULL`.  
`CV_ILL_INPUT` One of the input tolerances was negative.

#### **CVodeQuadSVtolerances**

Call `flag = CVodeQuadSVtolerances(cnode_mem, reltolQ, abstolQ);`

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

Arguments `cnode_mem` (`void *`) pointer to the CVODES memory block.  
`reltolQ` (`realtype`) is the scalar relative error tolerance.  
`abstolQ` (`N_Vector`) is the vector absolute error tolerance.

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

`CV_SUCCESS` The optional value has been successfully set.  
`CV_NO_QUAD` Quadrature integration was not initialized.  
`CV_MEM_NULL` The `cnode_mem` pointer is `NULL`.  
`CV_ILL_INPUT` One of the input tolerances was negative.

### 4.7.5 Optional outputs for quadrature integration

CVODES provides the following functions that can be used to obtain solver performance information related to quadrature integration.

#### **CVodeGetQuadNumRhsEvals**

Call `flag = CVodeGetQuadNumRhsEvals(cnode_mem, &nfQevals);`

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

Arguments `cnode_mem` (`void *`) pointer to the CVODES memory block.  
`nfQevals` (`long int`) number of calls made to the user's `fQ` function.

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

`CV_SUCCESS` The optional output value has been successfully set.  
`CV_MEM_NULL` The `cnode_mem` pointer is `NULL`.  
`CV_NO_QUAD` Quadrature integration has not been initialized.

#### **CVodeGetQuadNumErrTestFails**

Call `flag = CVodeGetQuadNumErrTestFails(cnode_mem, &nGetfails);`

Description The function `CVodeGetQuadNumErrTestFails` returns the number of local error test failures due to quadrature variables.

Arguments `cnode_mem` (`void *`) pointer to the CVODES memory block.  
`nGetfails` (`long int`) number of error test failures due to quadrature variables.

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

`CV_SUCCESS` The optional output value has been successfully set.  
`CV_MEM_NULL` The `cnode_mem` pointer is `NULL`.  
`CV_NO_QUAD` Quadrature integration has not been initialized.

**CVodeGetQuadErrWeights**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetQuadErrWeights(cvode_mem, eQweight);</code>  |
| Description  | The function <code>CVodeGetQuadErrWeights</code> returns the quadrature error weights at the current time.  |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>eQweight</code> (N_Vector) quadrature error weights at the current time.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_QUAD</code> Quadrature integration has not been initialized. |
| Notes        | The user must allocate memory for <code>eQweight</code> .<br><br>If quadratures were not included in the error control mechanism (through a call to <code>CVodeSetQuadErrCon</code> with <code>errconQ = SUNTRUE</code> ), <code>CVodeGetQuadErrWeights</code> does not set the <code>eQweight</code> vector.               |

**CVodeGetQuadStats**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetQuadStats(cvode_mem, &amp;nfQevals, &amp;nQetfails);</code>  |
| Description  | The function <code>CVodeGetQuadStats</code> returns the CVODES integrator statistics as a group.  |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>nfQevals</code> (long int) number of calls to the user's <code>fQ</code> function.<br><code>nQetfails</code> (long int) number of error test failures due to quadrature variables.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> the optional output values have been successfully set.<br><code>CV_MEM_NULL</code> the <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_QUAD</code> Quadrature integration has not been initialized. |

#### 4.7.6 User-supplied function for quadrature integration

For integration of quadrature equations, the user must provide a function that defines the right-hand side of the quadrature equations (in other words, the integrand function of the integral that must be evaluated). This function must be of type `CVQuadRhsFn` defined as follows:

**CVQuadRhsFn**

|              |   |
|--------------|---|
| Definition   | <code>typedef int (*CVQuadRhsFn)(realtype t, N_Vector y,<br/>N_Vector yQdot, void *user_data);</code>   |
| Purpose      | This function computes the quadrature equation right-hand side for a given value of the independent variable $t$ and state vector $y$ .   |
| Arguments    | <code>t</code> is the current value of the independent variable.<br><code>y</code> is the current value of the dependent variable vector, $y(t)$ .<br><code>yQdot</code> is the output vector $f_Q(t, y)$ .<br><code>user_data</code> is the <code>user_data</code> pointer passed to <code>CVodeSetUserData</code> . |
| Return value | A <code>CVQuadRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_QRHSFUNC_FAIL</code> is returned).                    |



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

Both `y` and `yQdot` are of type `N_Vector`, but they typically have different internal representations. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each `NVECTOR` implementation). For the sake of computational efficiency, the vector functions in the two `NVECTOR` implementations provided with `CVODES` do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

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

## 4.8 Preconditioner modules

The efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. For problems in which the user cannot define a more effective, problem-specific preconditioner, `CVODES` provides a banded preconditioner in the module `CVBANDPRE` and a band-block-diagonal preconditioner module `CVBBDPRE`.

### 4.8.1 A serial banded preconditioner module

This preconditioner provides a band matrix preconditioner for use with 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 `cvodes_bandpre.h` which declares the needed function prototypes. The following is a summary of the usage of this module. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. Initialize multi-threaded environment, if appropriate
2. Set problem dimensions
3. Set vector of initial values
4. Create `CVODES` object
5. Initialize `CVODES` 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:

|                       |  |
|-----------------------|--|
| <b>CVBandPrecInit</b> |  |
| Call                  | <code>flag = CVBandPrecInit(cvode_mem, N, mu, m1);</code>  |
| 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 CVODES memory block.<br><code>N</code> (sunindextype) problem dimension.<br><code>mu</code> (sunindextype) upper half-bandwidth of the Jacobian approximation.<br><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<br><code>CVSPILS_SUCCESS</code> The call to <code>CVBandPrecInit</code> was successful.<br><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.<br><code>CVSPILS_MEM_FAIL</code> A memory allocation request has failed.<br><code>CVSPILS_LMEM_NULL</code> A CVSPILS linear solver memory was not attached.<br><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    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>lenrwBP</code> (long int) the number of <b>realtype</b> values in the CVBANDPRE workspace.</p> <p><code>leniwBP</code> (long int) the number of integer values in the CVBANDPRE workspace.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CVSPILS_SUCCESS</code> The optional output values have been successfully set.</p> <p><code>CVSPILS_PMEM_NULL</code> The CVBANDPRE preconditioner has not been initialized.</p>   |
| Notes        | <p>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).</p> <p>The workspaces referred to here exist in addition to those given by the corresponding function <code>CVSpilsGetWorkSpace</code>.</p> |

**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    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>nfevalsBP</code> (long int) the number of calls to the user right-hand side function.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CVSPILS_SUCCESS</code> The optional output value has been successfully set.</p> <p><code>CVSPILS_PMEM_NULL</code> The CVBANDPRE preconditioner has not been initialized.</p>  |
| Notes        | <p>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.</p> |

### 4.8.2 A parallel band-block-diagonal preconditioner module

A principal reason for using a parallel ODE solver such as CVODES lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (2.5) 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 [24] and is included in a software module within the CVODES package. This module works with the parallel vector module `NVECTOR_PARALLEL` and is usable with any of the Krylov iterative linear solvers through the `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 `cfn`, and that are then used by `gloc`, which should not do any communication.

#### CVLocalFn

|            |   |   |
|------------|---|---|
| Definition | <pre>typedef int (*CVLocalFn)(sunindextype Nlocal, realtype t, N_Vector y,                         N_Vector glocal, void *user_data);</pre>       |   |
| Purpose    | This <code>gloc</code> function computes $g(t, y)$ . It loads the vector <code>glocal</code> as a function of <code>t</code> and <code>y</code> . |   |
| Arguments  | <code>Nlocal</code>   | is the local vector length.               |
|            | <code>t</code>  | is the value of the independent variable. |
|            | <code>y</code>  | is the dependent variable.                |

|              |   |
|--------------|---|
|              | <code>glocal</code> is the output vector.   |
|              | <code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> .  |
| Return value | A <code>CVLocalFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODES</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CVode</code> returns <code>CV_LSETUP_FAIL</code> ). |
| Notes        | This function must assume that all interprocess communication of data needed to calculate <code>glocal</code> has already been done, and that this data is accessible within <code>user_data</code> .<br>The case where $g$ is mathematically identical to $f$ is allowed.  |

|                 |
|-----------------|
| <b>CVCommFn</b> |
|-----------------|

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

Besides the header files required for the integration of the ODE problem (see §4.3), to use the `CVBBDPRE` module, the main program must include the header file `cvodes.bbdpre.h` which declares the needed function prototypes.

The following is a summary of the proper usage of this module. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. Initialize MPI environment
2. Set problem dimensions
3. Set vector of initial values
4. Create `CVODES` object
5. Initialize `CVODES` 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.

## 10. Attach linear solver module

Specify the upper and lower half-bandwidths `mudq` and `mldq`, and `mukeep` and `mlkeep`, and call

```
flag = CVBBDPrecInit(cvode_mem, local_N, mudq, mldq,
                    mukeep, mlkeep, dqrely, gloc, cfn);
```

## 12. Set linear solver interface optional inputs

### 13. Advance solution in time

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

15. Deallocate memory for solution vector

## 16. Free solver memory

## 17. Free linear solver memory

## 18. Finalize MPI

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

[illegible]

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

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

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

**mukeep** (**sunindextype**) upper half-bandwidth of the retained banded approximate Jacobian block.

**mlkeep** (sunindextype) lower half-bandwidth of the retained banded approximate Jacobian block.

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

**gloc** (CVLocalFn) the C function which computes the approximation  $g(t, y) \approx f(t, y)$ .

**cfn** (CVCmmFn) the optional C function which performs all interprocess communication required for the computation of  $g(t, y)$ .

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

**CVSPILS\_SUCCESS** The call to **CVBBDPrecInit** was successful.  
**CVSPILS\_MEM\_NULL** The **cvode\_mem** pointer was **NULL**.  
**CVSPILS\_MEM\_FAIL** A memory allocation request has failed.  
**CVSPILS\_LMEM\_NULL** A **CVSPILS** linear solver was not attached.  
**CVSPILS\_ILL\_INPUT** The supplied vector implementation was not compatible with block band preconditioner.

**Notes** If one of the half-bandwidths **mudq** or **mldq** to be used in the difference quotient calculation of the approximate Jacobian is negative or exceeds the value **local\_N-1**, it is replaced by 0 or **local\_N-1** accordingly.

The half-bandwidths **mudq** and **mldq** need not be the true half-bandwidths of the Jacobian of the local block of  $g$  when smaller values may provide a greater efficiency.

Also, the half-bandwidths **mukeep** and **mlkeep** of the retained banded approximate Jacobian block may be even smaller, to reduce storage and computational costs further.

For all four half-bandwidths, the values need not be the same on every processor.

The **CVBBDPRE** module also provides a reinitialization function to allow solving a sequence of problems of the same size, with the same linear solver choice, provided there is no change in **local\_N**, **mukeep**, or **mlkeep**. After solving one problem, and after calling **CVodeReInit** to re-initialize **CVODES** for a subsequent problem, a call to **CVBBDPrecReInit** can be made to change any of the following: the half-bandwidths **mudq** and **mldq** used in the difference-quotient Jacobian approximations, the relative increment **dqrely**, or one of the user-supplied functions **gloc** and **cfn**. If there is a change in any of the linear solver inputs, an additional call to the “Set” routines provided by the **SUNLINSOL** module, and/or one or more of the corresponding **CVSpilsSet\*\*\*** functions, must also be made (in the proper order).

#### CVBBDPrecReInit

**Call** **flag** = **CVBBDPrecReInit**(**cvode\_mem**, **mudq**, **mldq**, **dqrely**);

**Description** The function **CVBBDPrecReInit** re-initializes the **CVBBDPRE** preconditioner.

**Arguments** **cvode\_mem** (**void \***) pointer to the **CVODES** memory block.

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

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

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

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

**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         | <code>flag = CVBBDPrecGetWorkSpace(cvode_mem, &amp;lenrwBBDP, &amp;leniwBBDP);</code>  |
| Description  | The function <code>CVBBDPrecGetWorkSpace</code> returns the local CVBBDPRE real and integer workspace sizes.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>lenrwBBDP</code> (long int) local number of <b>realtype</b> values in the CVBBDPRE workspace.</p> <p><code>leniwBBDP</code> (long int) local number of integer values in the CVBBDPRE workspace.</p>   |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVSPILS_SUCCESS</code> The optional output value has been successfully set.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.</p> <p><code>CVSPILS_PMEM_NULL</code> The CVBBDPRE preconditioner has not been initialized.</p>                                    |
| Notes        | <p>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.</p> <p>The workspaces referred to here exist in addition to those given by the corresponding function <code>CVSpilsGetWorkSpace</code>.</p> |

**CVBBDPrecGetNumGfnEvals**

|              |   |
|--------------|---|
| Call         | <code>flag = CVBBDPrecGetNumGfnEvals(cvode_mem, &amp;ngevalsBBDP);</code>   |
| Description  | The function <code>CVBBDPrecGetNumGfnEvals</code> returns the number of calls made to the user-supplied <code>gloc</code> function due to the finite difference approximation of the Jacobian blocks used within the preconditioner setup function.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>ngevalsBBDP</code> (long int) the number of calls made to the user-supplied <code>gloc</code> function.</p>   |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVSPILS_SUCCESS</code> The optional output value has been successfully set.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.</p> <p><code>CVSPILS_PMEM_NULL</code> The CVBBDPRE preconditioner has not been initialized.</p> |

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 CVODES output and `npsolves` and `nfevalsLS` are linear solver optional outputs (see §4.5.8).



## Chapter 5

# Using CVODES for Forward Sensitivity Analysis

This chapter describes the use of CVODES to compute solution sensitivities using forward sensitivity analysis. One of our main guiding principles was to design the CVODES user interface for forward sensitivity analysis as an extension of that for IVP integration. Assuming a user main program and user-defined support routines for IVP integration have already been defined, in order to perform forward sensitivity analysis the user only has to insert a few more calls into the main program and (optionally) define an additional routine which computes the right-hand side of the sensitivity systems (2.11). The only departure from this philosophy is due to the `CVRhsFn` type definition (§4.6.1). Without changing the definition of this type, the only way to pass values of the problem parameters to the ODE right-hand side function is to require the user data structure `f_data` to contain a pointer to the array of real parameters  $p$ .

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

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable routines and of the user-supplied routines that were not already described in Chapter 4.

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

The following is a skeleton of the user's main program (or calling program) as an application of CVODES. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the `NVECTOR` implementation used; where this is not the case, refer to Chapter 7 for specifics. Differences between the user main program in §4.4 and the one below start only at step (13). Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

First, note that no additional header files need be included for forward sensitivity analysis beyond those for IVP solution (§4.4).

1. Initialize parallel or multi-threaded environment, if appropriate
2. Set problem dimensions etc.
3. Set vector of initial values
4. Create CVODES object
5. Initialize CVODES
6. Specify integration tolerances

7. Set optional inputs
8. Create matrix object
9. Create linear solver object
10. Set linear solver optional inputs
11. Attach linear solver module
12. Initialize quadrature problem, if not sensitivity-dependent
13. Define the sensitivity problem

- Number of sensitivities (required)

Set  $N_s = N_s$ , the number of parameters with respect to which sensitivities are to be computed.

- Problem parameters (optional)

If CVODES is to evaluate the right-hand sides of the sensitivity systems, set **p**, an array of  $N_p$  real parameters upon which the IVP depends. Only parameters with respect to which sensitivities are (potentially) desired need to be included. Attach **p** to the user data structure **user\_data**. For example, **user\_data->p = p**;

If the user provides a function to evaluate the sensitivity right-hand side, **p** need not be specified.

- Parameter list (optional)

If CVODES is to evaluate the right-hand sides of the sensitivity systems, set **plist**, an array of  $N_s$  integers to specify the parameters **p** with respect to which solution sensitivities are to be computed. If sensitivities with respect to the  $j$ -th parameter **p[j]** are desired ( $0 \leq j < N_p$ ), set  $plist_i = j$ , for some  $i = 0, \dots, N_s - 1$ .

If **plist** is not specified, CVODES will compute sensitivities with respect to the first  $N_s$  parameters; i.e.,  $plist_i = i$  ( $i = 0, \dots, N_s - 1$ ).

If the user provides a function to evaluate the sensitivity right-hand side, **plist** need not be specified.

- Parameter scaling factors (optional)

If CVODES is to estimate tolerances for the sensitivity solution vectors (based on tolerances for the state solution vector) or if CVODES is to evaluate the right-hand sides of the sensitivity systems using the internal difference-quotient function, the results will be more accurate if order of magnitude information is provided.

Set **pbar**, an array of  $N_s$  positive scaling factors. Typically, if  $p_i \neq 0$ , the value  $\bar{p}_i = |p_{plist_i}|$  can be used.

If **pbar** is not specified, CVODES will use  $\bar{p}_i = 1.0$ .

If the user provides a function to evaluate the sensitivity right-hand side and specifies tolerances for the sensitivity variables, **pbar** need not be specified.

Note that the names for **p**, **pbar**, **plist**, as well as the field **p** of **user\_data** are arbitrary, but they must agree with the arguments passed to **CVodeSetSensParams** below.

14. Set sensitivity initial conditions

Set the  $N_s$  vectors **yS0[i]** of initial values for sensitivities (for  $i = 0, \dots, N_s - 1$ ), using the appropriate functions defined by the particular NVECTOR implementation chosen.

First, create an array of  $N_s$  vectors by making the appropriate call

```
yS0 = N_VCloneVectorArray_***(Ns, y0);
```

or

```
yS0 = N_VCloneVectorArrayEmpty_***(Ns, y0);
```

Here the argument `y0` serves only to provide the `N_Vector` type for cloning.

Then, for each  $i = 0, \dots, N_s - 1$ , load initial values for the  $i$ -th sensitivity vector `yS0[i]`.

#### 15. Activate sensitivity calculations

Call `flag = CVodeSensInit` or `CVodeSensInit1` to activate forward sensitivity computations and allocate internal memory for CVODES related to sensitivity calculations (see §5.2.1).

#### 16. Set sensitivity tolerances

Call `CVodeSensSStolerances`, `CVodeSensSVtolerances` or `CVodeEETolerances`. (See §5.2.2).

#### 17. Set sensitivity analysis optional inputs

Call `CVodeSetSens*` routines to change from their default values any optional inputs that control the behavior of CVODES in computing forward sensitivities. (See §5.2.5.)

#### 18. Specify rootfinding

#### 19. Advance solution in time

#### 20. Extract sensitivity solution

After each successful return from `CVode`, the solution of the original IVP is available in the `y` argument of `CVode`, while the sensitivity solution can be extracted into `yS` (which can be the same as `yS0`) by calling one of the routines `CVodeGetSens`, `CVodeGetSens1`, `CVodeGetSensDky`, or `CVodeGetSensDky1` (see §5.2.4).

#### 21. Get optional outputs

#### 22. Deallocate memory for solution vector

#### 23. Deallocate memory for sensitivity vectors

Upon completion of the integration, deallocate memory for the vectors `yS0` using the appropriate destructor:

```
N_VDestroyVectorArray_***(yS0, Ns);
```

If `yS` was created from `realtype` arrays `yS_i`, it is the user's responsibility to also free the space for the arrays `yS0_i`.

#### 24. Free user data structure

#### 25. Free solver memory

#### 26. Free vector specification memory

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

#### 28. Finalize MPI, if used

## 5.2 User-callable routines for forward sensitivity analysis

This section describes the CVODES functions, in addition to those presented in §4.5, that are called by the user to setup and solve a forward sensitivity problem.

### 5.2.1 Forward sensitivity initialization and deallocation functions

Activation of forward sensitivity computation is done by calling `CVodeSensInit` or `CVodeSensInit1`, depending on whether the sensitivity right-hand side function returns all sensitivities at once or one by one, respectively. The form of the call to each of these routines is as follows:

#### `CVodeSensInit`

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSensInit(cvode_mem, Ns, ism, fS, yS0);</code>   |
| Description  | The routine <code>CVodeSensInit</code> activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.  |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>Ns</code> (<code>int</code>) the number of sensitivities to be computed.</p> <p><code>ism</code> (<code>int</code>) a flag used to select the sensitivity solution method. Its value can be <code>CV_SIMULTANEOUS</code> or <code>CV_STAGGERED</code>:</p> <ul style="list-style-type: none"> <li>• In the <code>CV_SIMULTANEOUS</code> approach, the state and sensitivity variables are corrected at the same time. If <code>CV_NEWTON</code> was selected as the non-linear system solution method, this amounts to performing a modified Newton iteration on the combined nonlinear system;</li> <li>• In the <code>CV_STAGGERED</code> approach, the correction step for the sensitivity variables takes place at the same time for all sensitivity equations, but only after the correction of the state variables has converged and the state variables have passed the local error test;</li> </ul> <p><code>fS</code> (<code>CVSensRhsFn</code>) is the C function which computes all sensitivity ODE right-hand sides at the same time. For full details see §5.3.</p> <p><code>yS0</code> (<code>N_Vector *</code>) a pointer to an array of <code>Ns</code> vectors containing the initial values of the sensitivities.</p> |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeSensInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODES memory block was not initialized through a previous call to <code>CVodeCreate</code>.</p> <p><code>CV_MEM_FAIL</code> A memory allocation request has failed.</p> <p><code>CV_ILL_INPUT</code> An input argument to <code>CVodeSensInit</code> has an illegal value.</p>  |
| Notes        | <p>Passing <code>fS=NULL</code> indicates using the default internal difference quotient sensitivity right-hand side routine.</p> <p>If an error occurred, <code>CVodeSensInit</code> also sends an error message to the error handler function.</p> <p>It is illegal here to use <code>ism = CV_STAGGERED1</code>. This option requires a different type for <code>fS</code> and can therefore only be used with <code>CVodeSensInit1</code> (see below).</p>  |



#### `CVodeSensInit1`

|             |   |
|-------------|---|
| Call        | <code>flag = CVodeSensInit1(cvode_mem, Ns, ism, fS1, yS0);</code>   |
| Description | The routine <code>CVodeSensInit1</code> activates forward sensitivity computations and allocates internal memory related to sensitivity calculations.   |
| Arguments   | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>Ns</code> (<code>int</code>) the number of sensitivities to be computed.</p> <p><code>ism</code> (<code>int</code>) a flag used to select the sensitivity solution method. Its value can be <code>CV_SIMULTANEOUS</code>, <code>CV_STAGGERED</code>, or <code>CV_STAGGERED1</code>:</p> |

- In the `CV_SIMULTANEOUS` approach, the state and sensitivity variables are corrected at the same time. If `CV_NEWTON` was selected as the nonlinear system solution method, this amounts to performing a modified Newton iteration on the combined nonlinear system;
- In the `CV_STAGGERED` approach, the correction step for the sensitivity variables takes place at the same time for all sensitivity equations, but only after the correction of the state variables has converged and the state variables have passed the local error test;
- In the `CV_STAGGERED1` approach, all corrections are done sequentially, first for the state variables and then for the sensitivity variables, one parameter at a time. If the sensitivity variables are not included in the error control, this approach is equivalent to `CV_STAGGERED`. Note that the `CV_STAGGERED1` approach can be used only if the user-provided sensitivity right-hand side function is of type `CVSensRhs1Fn` (see §5.3).

`fS1` (`CVSensRhs1Fn`) is the C function which computes the right-hand sides of the sensitivity ODE, one at a time. For full details see §5.3.

`yS0` (`N_Vector *`) a pointer to an array of `Ns` vectors containing the initial values of the sensitivities.

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

`CV_SUCCESS` The call to `CVodeSensInit1` was successful.

`CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.

`CV_MEM_FAIL` A memory allocation request has failed.

`CV_ILL_INPUT` An input argument to `CVodeSensInit1` has an illegal value.

Notes Passing `fS1=NULL` indicates using the default internal difference quotient sensitivity right-hand side routine.

If an error occurred, `CVodeSensInit1` also sends an error message to the error handler function.

In terms of the problem size  $N$ , number of sensitivity vectors  $N_s$ , and maximum method order `maxord`, the size of the real workspace is increased as follows:

- Base value:  $\text{lenrw} = \text{lenrw} + (\text{maxord}+5)N_sN$
- With `CVodeSensSVtolerances`:  $\text{lenrw} = \text{lenrw} + N_sN$

the size of the integer workspace is increased as follows:

- Base value:  $\text{leniw} = \text{leniw} + (\text{maxord}+5)N_sN_i$
- With `CVodeSensSVtolerances`:  $\text{leniw} = \text{leniw} + N_sN_i$

where  $N_i$  is the number of integers in one `N_Vector`.

The routine `CVodeSensReInit`, useful during the solution of a sequence of problems of same size, reinitializes the sensitivity-related internal memory. The call to it must follow a call to `CVodeSensInit` or `CVodeSensInit1` (and maybe a call to `CVodeReInit`). The number `Ns` of sensitivities is assumed to be unchanged since the call to the initialization function. The call to the `CVodeSensReInit` function has the form:

**CVodeSensReInit**

Call `flag = CVodeSensReInit(cvode_mem, ism, yS0);`

Description The routine `CVodeSensReInit` reinitializes forward sensitivity computations.

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

**ism** (int) a flag used to select the sensitivity solution method. Its value can be `CV_SIMULTANEOUS`, `CV_STAGGERED`, or `CV_STAGGERED1`.

**yS0** (`N_Vector *`) a pointer to an array of `Ns` variables of type `N_Vector` containing the initial values of the sensitivities.

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

**CV\_SUCCESS** The call to `CVodeReInit` was successful.

**CV\_MEM\_NULL** The CVODES memory block was not initialized through a previous call to `CVodeCreate`.

**CV\_NO\_SENS** Memory space for sensitivity integration was not allocated through a previous call to `CVodeSensInit`.

**CV\_ILL\_INPUT** An input argument to `CVodeSensReInit` has an illegal value.

**CV\_MEM\_FAIL** A memory allocation request has failed.

**Notes** All arguments of `CVodeSensReInit` are the same as those of the functions `CVodeSensInit` and `CVodeSensInit1`.

If an error occurred, `CVodeSensReInit` also sends a message to the error handler function.



The value of the input argument **ism** must be compatible with the type of the sensitivity ODE right-hand side function. Thus if the sensitivity module was initialized using `CVodeSensInit`, then it is illegal to pass `ism = CV_STAGGERED1` to `CVodeSensReInit`.

To deallocate all forward sensitivity-related memory (allocated in a prior call to `CVodeSensInit` or `CVodeSensInit1`), the user must call

#### `CVodeSensFree`

**Call** `CVodeSensFree(cvode_mem);`

**Description** The function `CVodeSensFree` frees the memory allocated for forward sensitivity computations by a previous call to `CVodeSensInit` or `CVodeSensInit1`.

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

**Return value** The function `CVodeSensFree` has no return value.

**Notes** In general, `CVodeSensFree` need not be called by the user, as it is invoked automatically by `CVodeFree`.

After a call to `CVodeSensFree`, forward sensitivity computations can be reactivated only by calling `CVodeSensInit` or `CVodeSensInit1` again.

To activate and deactivate forward sensitivity calculations for successive CVODES runs, without having to allocate and deallocate memory, the following function is provided:

#### `CVodeSensToggleOff`

**Call** `CVodeSensToggleOff(cvode_mem);`

**Description** The function `CVodeSensToggleOff` deactivates forward sensitivity calculations. It does *not* deallocate sensitivity-related memory.

**Arguments** `cvode_mem` (`void *`) pointer to the memory previously returned by `CVodeCreate`.

**Return value** The return value **flag** of `CVodeSensToggle` is one of:

**CV\_SUCCESS** `CVodeSensToggleOff` was successful.

**CV\_MEM\_NULL** `cvode_mem` was `NULL`.

**Notes** Since sensitivity-related memory is not deallocated, sensitivities can be reactivated at a later time (using `CVodeSensReInit`).

### 5.2.2 Forward sensitivity tolerance specification functions

One of the following three functions must be called to specify the integration tolerances for sensitivities. Note that this call must be made after the call to `CVodeSensInit`/`CVodeSensInit1`.

#### `CVodeSensSStolerances`

**Call** `flag = CVodeSensSStolerances(cvode_mem, reltolS, abstolS);`

**Description** The function `CVodeSensSStolerances` specifies scalar relative and absolute tolerances.

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.  
`reltolS` (`realtype`) is the scalar relative error tolerance.  
`abstolS` (`realtype*`) is a pointer to an array of length `Ns` containing the scalar absolute error tolerances, one for each parameter.

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

- `CV_SUCCESS` The call to `CVodeSStolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_SENS` The sensitivity allocation function (`CVodeSensInit` or `CVodeSensInit1`) has not been called.
- `CV_ILL_INPUT` One of the input tolerances was negative.

#### `CVodeSensSVtolerances`

**Call** `flag = CVodeSensSVtolerances(cvode_mem, reltolS, abstolS);`

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

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.  
`reltolS` (`realtype`) is the scalar relative error tolerance.  
`abstolS` (`N_Vector*`) is an array of `Ns` variables of type `N_Vector`. The `N_Vector` from `abstolS[is]` specifies the vector tolerances for `is`-th sensitivity.

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

- `CV_SUCCESS` The call to `CVodeSVtolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_SENS` The allocation function for sensitivities has not been called.
- `CV_ILL_INPUT` The relative error tolerance was negative or an absolute tolerance vector had a negative component.

**Notes** This choice of tolerances is important when the absolute error tolerance needs to be different for each component of any vector `yS[i]`.

#### `CVodeSensEETolerances`

**Call** `flag = CVodeSensEETolerances(cvode_mem);`

**Description** When `CVodeSensEETolerances` is called, CVODES will estimate tolerances for sensitivity variables based on the tolerances supplied for states variables and the scaling factors  $\bar{p}$ .

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

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

- `CV_SUCCESS` The call to `CVodeSensEETolerances` was successful.
- `CV_MEM_NULL` The CVODES memory block was not initialized through a previous call to `CVodeCreate`.
- `CV_NO_SENS` The sensitivity allocation function has not been called.

### 5.2.3 CVODES solver function

Even if forward sensitivity analysis was enabled, the call to the main solver function `CVode` is exactly the same as in §4.5.5. However, in this case the return value `flag` can also be one of the following:

|                                    |  |
|------------------------------------|--|
| <code>CV_SRHSFUNC_FAIL</code>      | The sensitivity right-hand side function failed in an unrecoverable manner.  |
| <code>CV_FIRST_SRHSFUNC_ERR</code> | The sensitivity right-hand side function failed at the first call.   |
| <code>CV_REPTD_SRHSFUNC_ERR</code> | Convergence tests occurred too many times due to repeated recoverable errors in the sensitivity right-hand side function. This flag will also be returned if the sensitivity right-hand side function had repeated recoverable errors during the estimation of an initial step size. |
| <code>CV_UNREC_SRHSFUNC_ERR</code> | The sensitivity right-hand function had a recoverable error, but no recovery was possible. This failure mode is rare, as it can occur only if the sensitivity right-hand side function fails recoverably after an error test failed while at order one.                              |

### 5.2.4 Forward sensitivity extraction functions

If forward sensitivity computations have been initialized by a call to `CVodeSensInit`/`CVodeSensInit1`, or reinitialized by a call to `CVSensReInit`, then CVODES computes both a solution and sensitivities at time `t`. However, `CVode` will still return only the solution  $y$  in `yout`. Solution sensitivities can be obtained through one of the following functions:

#### CVodeGetSens

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetSens(cvode_mem, &amp;tret, yS);</code>   |
| Description  | The function <code>CVodeGetSens</code> returns the sensitivity solution vectors after a successful return from <code>CVode</code> .   |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the memory previously allocated by <code>CVodeInit</code> .<br><code>tret</code> (realtype *) the time reached by the solver (output).<br><code>yS</code> (N_Vector *) array of computed forward sensitivity vectors.  |
| Return value | The return value <code>flag</code> of <code>CVodeGetSens</code> is one of:<br><code>CV_SUCCESS</code> <code>CVodeGetSens</code> was successful.<br><code>CV_MEM_NULL</code> <code>cvode_mem</code> was NULL.<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized.<br><code>CV_BAD_DKY</code> <code>yS</code> is NULL. |
| Notes        | Note that the argument <code>tret</code> is an output for this function. Its value will be the same as that returned at the last <code>CVode</code> call.   |

The function `CVodeGetSensDky` computes the  $k$ -th derivatives of the interpolating polynomials for the sensitivity variables at time `t`. This function is called by `CVodeGetSens` with `k = 0`, but may also be called directly by the user.

#### CVodeGetSensDky

|             |  |
|-------------|--|
| Call        | <code>flag = CVodeGetSensDky(cvode_mem, t, k, dkyS);</code>  |
| Description | The function <code>CVodeGetSensDky</code> returns derivatives of the sensitivity solution vectors after a successful return from <code>CVode</code> .  |
| Arguments   | <code>cvode_mem</code> (void *) pointer to the memory previously allocated by <code>CVodeInit</code> .<br><code>t</code> (realtype) specifies the time at which sensitivity information is requested. The time <code>t</code> must fall within the interval defined by the last successful step taken by CVODES.<br><code>k</code> (int) order of derivatives. |



**dkyS** (N\_Vector \*) array of  $N_s$  vectors containing the derivatives on output. The space for **dkyS** must be allocated by the user.

**Return value** The return value **flag** of **CVodeGetSensDky** is one of:

**CV\_SUCCESS** **CVodeGetSensDky** succeeded.  
**CV\_MEM\_NULL** **cvode\_mem** was NULL.  
**CV\_NO\_SENS** Forward sensitivity analysis was not initialized.  
**CV\_BAD\_DKY** One of the vectors **dkyS** is NULL.  
**CV\_BAD\_K** **k** is not in the range  $0, 1, \dots, q_{\text{last}}$ .  
**CV\_BAD\_T** The time **t** is not in the allowed range.

Forward sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions **CVodeGetSens1** and **CVodeGetSensDky1**, defined as follows:

#### **CVodeGetSens1**

**Call** **flag** = **CVodeGetSens1**(**cvode\_mem**, &**tret**, **is**, **yS**);

**Description** The function **CVodeGetSens1** returns the **is**-th sensitivity solution vector after a successful return from **CVode**.

**Arguments** **cvode\_mem** (void \*) pointer to the memory previously allocated by **CVodeInit**.  
**tret** (realtype \*) the time reached by the solver (output).  
**is** (int) specifies which sensitivity vector is to be returned ( $0 \leq \text{is} < N_s$ ).  
**yS** (N\_Vector) the computed forward sensitivity vector.

**Return value** The return value **flag** of **CVodeGetSens1** is one of:

**CV\_SUCCESS** **CVodeGetSens1** was successful.  
**CV\_MEM\_NULL** **cvode\_mem** was NULL.  
**CV\_NO\_SENS** Forward sensitivity analysis was not initialized.  
**CV\_BAD\_IS** The index **is** is not in the allowed range.  
**CV\_BAD\_DKY** **yS** is NULL.  
**CV\_BAD\_T** The time **t** is not in the allowed range.

**Notes** Note that the argument **tret** is an output for this function. Its value will be the same as that returned at the last **CVode** call.

#### **CVodeGetSensDky1**

**Call** **flag** = **CVodeGetSensDky1**(**cvode\_mem**, **t**, **k**, **is**, **dkyS**);

**Description** The function **CVodeGetSensDky1** returns the **k**-th derivative of the **is**-th sensitivity solution vector after a successful return from **CVode**.

**Arguments** **cvode\_mem** (void \*) pointer to the memory previously allocated by **CVodeInit**.  
**t** (realtype) specifies the time at which sensitivity information is requested. The time **t** must fall within the interval defined by the last successful step taken by **CVODES**.  
**k** (int) order of derivative.  
**is** (int) specifies the sensitivity derivative vector to be returned ( $0 \leq \text{is} < N_s$ ).  
**dkyS** (N\_Vector) the vector containing the derivative. The space for **dkyS** must be allocated by the user.

**Return value** The return value **flag** of **CVodeGetSensDky1** is one of:

**CV\_SUCCESS** **CVodeGetQuadDky1** succeeded.  
**CV\_MEM\_NULL** The pointer to **cvode\_mem** was NULL.  
**CV\_NO\_SENS** Forward sensitivity analysis was not initialized.

CV\_BAD\_DKY    dkyS or one of the vectors dkyS[i] is NULL.  
 CV\_BAD\_IS    The index *is* is not in the allowed range.  
 CV\_BAD\_K    *k* is not in the range 0, 1, ..., *qlast*.  
 CV\_BAD\_T    The time *t* is not in the allowed range.

### 5.2.5 Optional inputs for forward sensitivity analysis

Optional input variables that control the computation of sensitivities can be changed from their default values through calls to `CVodeSetSens*` functions. Table 5.1 lists all forward sensitivity optional input functions in CVODES which are described in detail in the remainder of this section.


#### CVodeSetSensParams

**Call**            `flag = CVodeSetSensParams(cvode_mem, p, pbar, plist);`

**Description**    The function `CVodeSetSensParams` specifies problem parameter information for sensitivity calculations.

**Arguments**    `cvode_mem` (void \*) pointer to the CVODES memory block.  
                  `p`            (realtype \*) a pointer to the array of real problem parameters used to evaluate  $f(t, y, p)$ . If non-NULL, `p` must point to a field in the user's data structure `user_data` passed to the right-hand side function. (See §5.1).  
                  `pbar`        (realtype \*) an array of *Ns* positive scaling factors. If non-NULL, `pbar` must have all its components > 0.0. (See §5.1).  
                  `plist`        (int \*) an array of *Ns* non-negative indices to specify which components `p[i]` to use in estimating the sensitivity equations. If non-NULL, `plist` must have all components  $\geq 0$ . (See §5.1).

**Return value**    The return value `flag` (of type `int`) is one of:  
                  `CV_SUCCESS`    The optional value has been successfully set.  
                  `CV_MEM_NULL`    The `cvode_mem` pointer is NULL.  
                  `CV_NO_SENS`    Forward sensitivity analysis was not initialized.  
                  `CV_ILL_INPUT`    An argument has an illegal value.

 **Notes**            This function must be preceded by a call to `CVodeSensInit` or `CVodeSensInit1`.

#### CVodeSetSensDQMethod

**Call**            `flag = CVodeSetSensDQMethod(cvode_mem, DQtype, DQrhmax);`

**Description**    The function `CVodeSetSensDQMethod` specifies the difference quotient strategy in the case in which the right-hand side of the sensitivity equations are to be computed by CVODES.

**Arguments**    `cvode_mem` (void \*) pointer to the CVODES memory block.  
                  `DQtype`        (int) specifies the difference quotient type. Its value can be `CV_CENTERED` or `CV_FORWARD`.

Table 5.1: Forward sensitivity optional inputs

| Optional input                      | Routine name                            | Default      |
|-------------------------------------|---|--------------|
| Sensitivity scaling factors         | <code>CVodeSetSensParams</code>         | NULL         |
| DQ approximation method             | <code>CVodeSetSensDQMethod</code>       | centered/0.0 |
| Error control strategy              | <code>CVodeSetSensErrCon</code>         | SUNFALSE     |
| Maximum no. of nonlinear iterations | <code>CVodeSetSensMaxNonlinIters</code> | 3            |

|              |  |
|--------------|--|
|              | <b>DQrhomax</b> ( <b>realtype</b> ) positive value of the selection parameter used in deciding switching between a simultaneous or separate approximation of the two terms in the sensitivity right-hand side.   |
| Return value | The return value <b>flag</b> (of type <b>int</b> ) is one of:<br><b>CV_SUCCESS</b> The optional value has been successfully set.<br><b>CV_MEM_NULL</b> The <b>cvode_mem</b> pointer is <b>NULL</b> .<br><b>CV_ILL_INPUT</b> An argument has an illegal value.  |
| Notes        | If <b>DQrhomax</b> = 0.0, then no switching is performed. The approximation is done simultaneously using either centered or forward finite differences, depending on the value of <b>DQtype</b> . For values of <b>DQrhomax</b> $\geq$ 1.0, the simultaneous approximation is used whenever the estimated finite difference perturbations for states and parameters are within a factor of <b>DQrhomax</b> , and the separate approximation is used otherwise. Note that a value <b>DQrhomax</b> < 1.0 will effectively disable switching. See §2.6 for more details.<br>The default value are <b>DQtype</b> = <b>CV_CENTERED</b> and <b>DQrhomax</b> = 0.0. |

#### CVodeSetSensErrCon

|              |  |
|--------------|--|
| Call         | <b>flag</b> = <b>CVodeSetSensErrCon</b> ( <b>cvode_mem</b> , <b>errconS</b> );   |
| Description  | The function <b>CVodeSetSensErrCon</b> specifies the error control strategy for sensitivity variables.   |
| Arguments    | <b>cvode_mem</b> ( <b>void *</b> ) pointer to the CVODES memory block.<br><b>errconS</b> ( <b>booleantype</b> ) specifies whether sensitivity variables are to be included ( <b>SUNTRUE</b> ) or not ( <b>SUNFALSE</b> ) in the error control mechanism.   |
| Return value | The return value <b>flag</b> (of type <b>int</b> ) is one of:<br><b>CV_SUCCESS</b> The optional value has been successfully set.<br><b>CV_MEM_NULL</b> The <b>cvode_mem</b> pointer is <b>NULL</b> .   |
| Notes        | By default, <b>errconS</b> is set to <b>SUNFALSE</b> . If <b>errconS</b> = <b>SUNTRUE</b> then both state variables and sensitivity variables are included in the error tests. If <b>errconS</b> = <b>SUNFALSE</b> then the sensitivity variables are excluded from the error tests. Note that, in any event, all variables are considered in the convergence tests. |

#### CVodeSetSensMaxNonlinIters

|              |  |
|--------------|--|
| Call         | <b>flag</b> = <b>CVodeSetSensMaxNonlinIters</b> ( <b>cvode_mem</b> , <b>maxcorS</b> );   |
| Description  | The function <b>CVodeSetSensMaxNonlinIters</b> specifies the maximum number of nonlinear solver iterations for sensitivity variables per step.   |
| Arguments    | <b>cvode_mem</b> ( <b>void *</b> ) pointer to the CVODES memory block.<br><b>maxcorS</b> ( <b>int</b> ) maximum number of nonlinear solver iterations allowed per step (> 0).                        |
| Return value | The return value <b>flag</b> (of type <b>int</b> ) is one of:<br><b>CV_SUCCESS</b> The optional value has been successfully set.<br><b>CV_MEM_NULL</b> The <b>cvode_mem</b> pointer is <b>NULL</b> . |
| Notes        | The default value is 3.  |

### 5.2.6 Optional outputs for forward sensitivity analysis

Optional output functions that return statistics and solver performance information related to forward sensitivity computations are listed in Table 5.2 and described in detail in the remainder of this section.

**CVodeGetSensNumRhsEvals**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetSensNumRhsEvals(cvode_mem, &amp;nfSevals);</code>  |
| Description  | The function <code>CVodeGetSensNumRhsEvals</code> returns the number of calls to the sensitivity right-hand side function.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nfSevals</code> ( <code>long int</code> ) number of calls to the sensitivity right-hand side function.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized.  |
| Notes        | In order to accommodate any of the three possible sensitivity solution methods, the default internal finite difference quotient functions evaluate the sensitivity right-hand sides one at a time. Therefore, <code>nfSevals</code> will always be a multiple of the number of sensitivity parameters (the same as the case in which the user supplies a routine of type <code>CVSensRhs1Fn</code> ). |

**CVodeGetNumRhsEvalsSens**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetNumRhsEvalsSens(cvode_mem, &amp;nfevalsS);</code>   |
| Description  | The function <code>CVodeGetNumRhsEvalsSens</code> returns the number of calls to the user's right-hand side function due to the internal finite difference approximation of the sensitivity right-hand sides.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nfevalsS</code> ( <code>long int</code> ) number of calls to the user's ODE right-hand side function for the evaluation of sensitivity right-hand sides.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized. |
| Notes        | This counter is incremented only if the internal finite difference approximation routines are used for the evaluation of the sensitivity right-hand sides.   |

**CVodeGetSensNumErrTestFails**

|      |   |
|------|---|
| Call | <code>flag = CVodeGetSensNumErrTestFails(cvode_mem, &amp;nSetfails);</code> |
|------|---|

Table 5.2: Forward sensitivity optional outputs

| Optional output                                    | Routine name  |
|--|---|
| No. of calls to sensitivity r.h.s. function        | <code>CVodeGetSensNumRhsEvals</code>                |
| No. of calls to r.h.s. function for sensitivity    | <code>CVodeGetNumRhsEvalsSens</code>                |
| No. of sensitivity local error test failures       | <code>CVodeGetSensNumErrTestFails</code>            |
| No. of calls to lin. solv. setup routine for sens. | <code>CVodeGetSensNumLinSolvSetups</code>           |
| Error weight vector for sensitivity variables      | <code>CVodeGetSensErrWeights</code>                 |
| No. of sens. nonlinear solver iterations           | <code>CVodeGetSensNumNonlinSolvIters</code>         |
| No. of sens. convergence failures                  | <code>CVodeGetSensNumNonlinSolvConvFails</code>     |
| No. of staggered nonlinear solver iterations       | <code>CVodeGetStgrSensNumNonlinSolvIters</code>     |
| No. of staggered convergence failures              | <code>CVodeGetStgrSensNumNonlinSolvConvFails</code> |

|              |  |
|--------------|--|
| Description  | The function <code>CVodeGetSensNumErrTestFails</code> returns the number of local error test failures for the sensitivity variables that have occurred.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nSetfails</code> ( <code>long int</code> ) number of error test failures.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized. |
| Notes        | This counter is incremented only if the sensitivity variables have been included in the error test (see <code>CVodeSetSensErrCon</code> in §5.2.5). Even in that case, this counter is not incremented if the <code>ism=CV_SIMULTANEOUS</code> sensitivity solution method has been used.  |

**CVodeGetSensNumLinSolvSetups**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetSensNumLinSolvSetups(cvode_mem, &amp;nlinsetupsS);</code>   |
| Description  | The function <code>CVodeGetSensNumLinSolvSetups</code> returns the number of calls to the linear solver setup function due to forward sensitivity calculations.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nlinsetupsS</code> ( <code>long int</code> ) number of calls to the linear solver setup function.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized. |
| Notes        | This counter is incremented only if Newton iteration has been used and if either the <code>ism = CV_STAGGERED</code> or the <code>ism = CV_STAGGERED1</code> sensitivity solution method has been specified (see §5.2.1).  |

**CVodeGetSensStats**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetSensStats(cvode_mem, &amp;nfSevals, &amp;nfevalsS, &amp;nSetfails, &amp;nSetfails, &amp;nlinsetupsS);</code>  |
| Description  | The function <code>CVodeGetSensStats</code> returns all of the above sensitivity-related solver statistics as a group.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nfSevals</code> ( <code>long int</code> ) number of calls to the sensitivity right-hand side function.<br><code>nfevalsS</code> ( <code>long int</code> ) number of calls to the ODE right-hand side function for sensitivity evaluations.<br><code>nSetfails</code> ( <code>long int</code> ) number of error test failures.<br><code>nlinsetupsS</code> ( <code>long int</code> ) number of calls to the linear solver setup function. |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><br><code>CV_SUCCESS</code> The optional output values have been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized.   |

**CVodeGetSensErrWeights**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetSensErrWeights(cvode_mem, eSweight);</code>   |
| Description  | The function <code>CVodeGetSensErrWeights</code> returns the sensitivity error weight vectors at the current time. These are the reciprocals of the $W_i$ of (2.7) for the sensitivity variables.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>eSweight</code> ( <code>N_Vector *</code> ) pointer to the array of error weight vectors.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized. |
| Notes        | The user must allocate memory for <code>eweightS</code> .  |

**CVodeGetSensNumNonlinSolvIters**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetSensNumNonlinSolvIters(cvode_mem, &amp;nSniters);</code>   |
| Description  | The function <code>CVodeGetSensNumNonlinSolvIters</code> returns the number of nonlinear iterations performed for sensitivity calculations.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nSniters</code> ( <code>long int</code> ) number of nonlinear iterations performed.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized.  |
| Notes        | This counter is incremented only if <code>ism</code> was <code>CV_STAGGERED</code> or <code>CV_STAGGERED1</code> (see §5.2.1).<br><br>In the <code>CV_STAGGERED1</code> case, the value of <code>nSniters</code> is the sum of the number of nonlinear iterations performed for each sensitivity equation. These individual counters can be obtained through a call to <code>CVodeGetStgrSensNumNonlinSolvIters</code> (see below). |

**CVodeGetSensNumNonlinSolvConvFails**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeGetSensNumNonlinSolvConvFails(cvode_mem, &amp;nSncfails);</code>  |
| Description  | The function <code>CVodeGetSensNumNonlinSolvConvFails</code> returns the number of nonlinear convergence failures that have occurred for sensitivity calculations.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nSncfails</code> ( <code>long int</code> ) number of nonlinear convergence failures.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Forward sensitivity analysis was not initialized.  |
| Notes        | This counter is incremented only if <code>ism</code> was <code>CV_STAGGERED</code> or <code>CV_STAGGERED1</code> (see §5.2.1).<br><br>In the <code>CV_STAGGERED1</code> case, the value of <code>nSncfails</code> is the sum of the number of non-linear convergence failures that occurred for each sensitivity equation. These individual counters can be obtained through a call to <code>CVodeGetStgrSensNumNonlinConvFails</code> (see below). |

**CVodeGetSensNonlinSolvStats**

**Call** `flag = CVodeGetSensNonlinSolvStats(cvode_mem, &nSniters, &nSncfails);`

**Description** The function `CVodeGetSensNonlinSolvStats` returns the sensitivity-related nonlinear solver statistics as a group.

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nSniters` (`long int`) number of nonlinear iterations performed.  
`nSncfails` (`long int`) number of nonlinear convergence failures.

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

`CV_SUCCESS` The optional output values have been successfully set.  
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.  
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

**CVodeGetStgrSensNumNonlinSolvIters**

**Call** `flag = CVodeGetStgrSensNumNonlinSolvIters(cvode_mem, nSTGR1niters);`

**Description** The function `CVodeGetStgrSensNumNonlinSolvIters` returns the number of nonlinear (functional or Newton) iterations performed for each sensitivity equation separately, in the `CV_STAGGERED1` case.

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nSTGR1niters` (`long int *`) an array (of dimension `Ns`) which will be set with the number of nonlinear iterations performed for each sensitivity system individually.

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

`CV_SUCCESS` The optional output value has been successfully set.  
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.  
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

**Notes** The user must allocate space for `nSTGR1niters`.

**CVodeGetStgrSensNumNonlinSolvConvFails**

**Call** `flag = CVodeGetStgrSensNumNonlinSolvConvFails(cvode_mem, nSTGR1ncfails);`

**Description** The function `CVodeGetStgrSensNumNonlinSolvConvFails` returns the number of nonlinear convergence failures that have occurred for each sensitivity equation separately, in the `CV_STAGGERED1` case.

**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nSTGR1ncfails` (`long int *`) an array (of dimension `Ns`) which will be set with the number of nonlinear convergence failures for each sensitivity system individually.

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

`CV_SUCCESS` The optional output value has been successfully set.  
`CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.  
`CV_NO_SENS` Forward sensitivity analysis was not initialized.

**Notes** The user must allocate space for `nSTGR1ncfails`.



## 5.3 User-supplied routines for forward sensitivity analysis

In addition to the required and optional user-supplied routines described in §4.6, when using CVODES for forward sensitivity analysis, the user has the option of providing a routine that calculates the right-hand side of the sensitivity equations (2.11).

By default, CVODES uses difference quotient approximation routines for the right-hand sides of the sensitivity equations. However, CVODES allows the option for user-defined sensitivity right-hand side routines (which also provides a mechanism for interfacing CVODES to routines generated by automatic differentiation).

### 5.3.1 Sensitivity equations right-hand side (all at once)

If the CV\_SIMULTANEOUS or CV\_STAGGERED approach was selected in the call to C\_VodeSensInit or C\_VodeSensInit1, the user may provide the right-hand sides of the sensitivity equations (2.11), for all sensitivity parameters at once, through a function of type CVSensRhsFn defined by:

**CVSensRhsFn**

|              |   |
|--------------|---|
| Definition   | <pre>typedef int (*CVSensRhsFn)(int Ns, realtype t,                            N_Vector y, N_Vector ydot,                            N_Vector *yS, N_Vector *ySdot,                            void *user_data,                            N_Vector tmp1, N_Vector tmp2);</pre>   |
| Purpose      | This function computes the sensitivity right-hand side for all sensitivity equations at once. It must compute the vectors $(\partial f/\partial y)s_i(t) + (\partial f/\partial p_i)$ and store them in <code>ySdot[i]</code> .   |
| Arguments    | <p><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the state vector, <math>y(t)</math>.</p> <p><code>ydot</code> is the current value of the right-hand side of the state equations.</p> <p><code>yS</code> contains the current values of the sensitivity vectors.</p> <p><code>ySdot</code> is the output of <code>CVSensRhsFn</code>. On exit it must contain the sensitivity right-hand side vectors.</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> <p><code>tmp1</code></p> <p><code>tmp2</code> are <code>N_Vectors</code> of length <math>N</math> which can be used as temporary storage.</p> |
| Return value | A <code>CVSensRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODES</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_SRHSFUNC_FAIL</code> is returned).   |
| Notes        | A sensitivity right-hand side function of type <code>CVSensRhsFn</code> is not compatible with the <code>CV_STAGGERED1</code> approach.   |

There are two situations in which recovery is not possible even if CVSensRhsFn function returns a recoverable error flag. One is when this occurs at the very first call to the CVSensRhsFn (in which case CVODES returns CV\_FIRST\_SRHSFUNC\_ERR). The other is when a recoverable error is reported by CVSensRhsFn after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns CV\_UNREC\_SRHSFUNC\_ERR).



### 5.3.2 Sensitivity equations right-hand side (one at a time)

Alternatively, the user may provide the sensitivity right-hand sides, one sensitivity parameter at a time, through a function of type `CVSensRhs1Fn`. Note that a sensitivity right-hand side function of type `CVSensRhs1Fn` is compatible with any valid value of the argument `ism` to `CVodeSensInit` and `CVodeSensInit1`, and is *required* if `ism = CV_STAGGERED1` in the call to `CVodeSensInit1`. The type `CVSensRhs1Fn` is defined by

`CVSensRhs1Fn`

|              |  |
|--------------|--|
| Definition   | <pre>typedef int (*CVSensRhs1Fn)(int Ns, realtype t,                              N_Vector y, N_Vector ydot,                              int iS, N_Vector yS, N_Vector ySdot,                              void *user_data,                              N_Vector tmp1, N_Vector tmp2);</pre>   |
| Purpose      | This function computes the sensitivity right-hand side for one sensitivity equation at a time. It must compute the vector $(\partial f / \partial y) s_i(t) + (\partial f / \partial p_i)$ for $i = iS$ and store it in <code>ySdot</code> .   |
| Arguments    | <p><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the state vector, <math>y(t)</math>.</p> <p><code>ydot</code> is the current value of the right-hand side of the state equations.</p> <p><code>iS</code> is the index of the parameter for which the sensitivity right-hand side must be computed (<math>0 \leq iS &lt; Ns</math>).</p> <p><code>yS</code> contains the current value of the <math>iS</math>-th sensitivity vector.</p> <p><code>ySdot</code> is the output of <code>CVSensRhs1Fn</code>. On exit it must contain the <math>iS</math>-th sensitivity right-hand side 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> <p><code>tmp1</code><br/><code>tmp2</code> are <code>N_Vectors</code> of length <math>N</math> which can be used as temporary storage.</p> |
| Return value | A <code>CVSensRhs1Fn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODES</code> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_SRHSFUNC_FAIL</code> is returned).   |
| Notes        | <p>Allocation of memory for <code>ySdot</code> is handled within <code>CVODES</code>.</p> <p>There are two situations in which recovery is not possible even if <code>CVSensRhs1Fn</code> function returns a recoverable error flag. One is when this occurs at the very first call to the <code>CVSensRhs1Fn</code> (in which case <code>CVODES</code> returns <code>CV_FIRST_SRHSFUNC_ERR</code>). The other is when a recoverable error is reported by <code>CVSensRhs1Fn</code> after an error test failure, while the linear multistep method order equal to 1 (in which case <code>CVODES</code> returns <code>CV_UNREC_SRHSFUNC_ERR</code>).</p>  |

## 5.4 Integration of quadrature equations depending on forward sensitivities

`CVODES` provides support for integration of quadrature equations that depends not only on the state variables but also on forward sensitivities.

The following is an overview of the sequence of calls in a user's main program in this situation. Steps that are unchanged from the skeleton program presented in §5.1 are grayed out.

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

2. Set problem dimensions etc.
3. Set vectors of initial values
4. Create CVODES object
5. Initialize CVODES
6. Specify integration tolerances
7. Set optional inputs
8. Create matrix object
9. Create linear solver object
10. Set linear solver optional inputs
11. Initialize sensitivity-independent quadrature problem
12. Define the sensitivity problem
13. Set sensitivity initial conditions
14. Activate sensitivity calculations
15. Set sensitivity analysis optional inputs
16. Set vector of initial values for quadrature variables  
Typically, the quadrature variables should be initialized to 0.
17. Initialize sensitivity-dependent quadrature integration  
Call `CVodeQuadSensInit` to specify the quadrature equation right-hand side function and to allocate internal memory related to quadrature integration. See §5.4.1 for details.
18. Set optional inputs for sensitivity-dependent quadrature integration  
Call `CVodeSetQuadSensErrCon` to indicate whether or not quadrature variables should be used in the step size control mechanism. If so, one of the `CVodeQuadSens*tolerances` functions must be called to specify the integration tolerances for quadrature variables. See §5.4.4 for details.
19. Advance solution in time
20. Extract sensitivity-dependent quadrature variables  
Call `CVodeGetQuadSens`, `CVodeGetQuadSens1`, `CVodeGetQuadSensDky` or `CVodeGetQuadSensDky1` to obtain the values of the quadrature variables or their derivatives at the current time. See §5.4.3 for details.
21. Get optional outputs
22. Extract sensitivity solution
23. Get sensitivity-dependent quadrature optional outputs  
Call `CVodeGetQuadSens*` functions to obtain desired optional output related to the integration of sensitivity-dependent quadratures. See §5.4.5 for details.
24. Deallocate memory for solutions vector
25. Deallocate memory for sensitivity vectors

26. Deallocate memory for sensitivity-dependent quadrature variables

27. Free vector specification memory

28. Free linear solver and matrix memory

29. Free solver memory

30. Finalize MPI, if used

Note: `CVodeQuadSensInit` (step 17 above) can be called and quadrature-related optional inputs (step 18 above) can be set anywhere between steps 12 and 19.

### 5.4.1 Sensitivity-dependent quadrature initialization and deallocation

The function `CVodeQuadSensInit` activates integration of quadrature equations depending on sensitivities and allocates internal memory related to these calculations. If `rhsQS` is input as `NULL`, then `CVODES` uses an internal function that computes difference quotient approximations to the functions  $\bar{q}_i = q_y s_i + q_{p_i}$ , in the notation of (2.9). The form of the call to this function is as follows:

| <div style="border: 1px solid black; padding: 2px; display: inline-block;">CVodeQuadSensInit</div> |   |
|--|---|
| Call   | <code>flag = CVodeQuadSensInit(cvode_mem, rhsQS, yQS0);</code>  |
| Description  | The function <code>CVodeQuadSensInit</code> provides required problem specifications, allocates internal memory, and initializes quadrature integration.  |
| Arguments  | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the <code>CVODES</code> memory block returned by <code>CVodeCreate</code>.</p> <p><code>rhsQS</code> (<code>CVQuadSensRhsFn</code>) is the C function which computes <math>f_{QS}</math>, the right-hand side of the sensitivity-dependent quadrature equations (for full details see §5.4.6).</p> <p><code>yQS0</code> (<code>N_Vector *</code>) contains the initial values of sensitivity-dependent quadratures.</p>  |
| Return value   | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeQuadSensInit</code> was successful.</p> <p><code>CVODE_MEM_NULL</code> The <code>CVODES</code> memory was not initialized by a prior call to <code>CVodeCreate</code>.</p> <p><code>CVODE_MEM_FAIL</code> A memory allocation request failed.</p> <p><code>CV_NO_SENS</code> The sensitivities were not initialized by a prior call to <code>CVodeSensInit</code> or <code>CVodeSensInit1</code>.</p> <p><code>CV_ILL_INPUT</code> The parameter <code>yQS0</code> is <code>NULL</code>.</p> |
| Notes  | <p>Before calling <code>CVodeQuadSensInit</code>, the user must enable the sensitivities by calling <code>CVodeSensInit</code> or <code>CVodeSensInit1</code>.</p> <p>If an error occurred, <code>CVodeQuadSensInit</code> also sends an error message to the error handler function.</p>   |



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

- Base value:  $\text{lenrw} = \text{lenrw} + (\text{maxord}+5)N_q$
- If `CVodeQuadSensSVtolerances` is called:  $\text{lenrw} = \text{lenrw} + N_q N_s$

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

- Base value:  $\text{leniw} = \text{leniw} + (\text{maxord}+5)N_q$
- If `CVodeQuadSensSVtolerances` is called:  $\text{leniw} = \text{leniw} + N_q N_s$

The function `CVodeQuadSensReInit`, useful during the solution of a sequence of problems of same size, reinitializes quadrature-related internal memory and must follow a call to `CVodeQuadSensInit`. The number `Nq` of quadratures as well as the number `Ns` of sensitivities are assumed to be unchanged from the prior call to `CVodeQuadSensInit`. The call to the `CVodeQuadSensReInit` function has the form:

#### `CVodeQuadSensReInit`

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeQuadSensReInit(cvode_mem, yQS0);</code>  |
| Description  | The function <code>CVodeQuadSensReInit</code> provides required problem specifications and reinitializes the sensitivity-dependent quadrature integration.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>yQS0</code> (N_Vector *) contains the initial values of sensitivity-dependent quadratures.</p>   |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeQuadSensReInit</code> was successful.</p> <p><code>CVODE_MEM_NULL</code> The CVODES memory was not initialized by a prior call to <code>CVodeCreate</code>.</p> <p><code>CV_NO_SENS</code> Memory space for the sensitivity calculation was not allocated by a prior call to <code>CVodeSensInit</code> or <code>CVodeSensInit1</code>.</p> <p><code>CV_NO_QUADSENS</code> Memory space for the sensitivity quadratures integration was not allocated by a prior call to <code>CVodeQuadSensInit</code>.</p> <p><code>CV_ILL_INPUT</code> The parameter <code>yQS0</code> is <code>NULL</code>.</p> |
| Notes        | If an error occurred, <code>CVodeQuadSensReInit</code> also sends an error message to the error handler function.  |

#### `CVodeQuadSensFree`

|              |   |
|--------------|---|
| Call         | <code>CVodeQuadSensFree(cvode_mem);</code>  |
| Description  | The function <code>CVodeQuadSensFree</code> frees the memory allocated for sensitivity quadrature integration.                        |
| Arguments    | The argument is the pointer to the CVODES memory block (of type <code>void *</code> ).  |
| Return value | The function <code>CVodeQuadSensFree</code> has no return value.  |
| Notes        | In general, <code>CVodeQuadSensFree</code> need not be called by the user, as it is invoked automatically by <code>CVodeFree</code> . |

### 5.4.2 CVODES solver function

Even if quadrature integration was enabled, the call to the main solver function `CVode` is exactly the same as in §4.5.5. However, in this case the return value `flag` can also be one of the following:

|                                     |  |
|-------------------------------------|--|
| <code>CV_QSRHSFUNC_ERR</code>       | The sensitivity quadrature right-hand side function failed in an unrecoverable manner.   |
| <code>CV_FIRST_QSRHSFUNC_ERR</code> | The sensitivity quadrature right-hand side function failed at the first call.  |
| <code>CV_REPTD_QSRHSFUNC_ERR</code> | Convergence test failures occurred too many times due to repeated recoverable errors in the quadrature right-hand side function. This flag will also be returned if the quadrature right-hand side function had repeated recoverable errors during the estimation of an initial step size (assuming the sensitivity quadrature variables are included in the error tests). |

### 5.4.3 Sensitivity-dependent quadrature extraction functions

If sensitivity-dependent quadratures have been initialized by a call to `CVodeQuadSensInit`, or reinitialized by a call to `CVodeQuadSensReInit`, then CVODES computes a solution, sensitivity vectors, and quadratures depending on sensitivities at time `t`. However, `CVode` will still return only the solution `y`. Sensitivity-dependent quadratures can be obtained using one of the following functions:

#### CVodeGetQuadSens

Call `flag = CVodeGetQuadSens(cvode_mem, &tret, yQS);`

Description The function `CVodeGetQuadSens` returns the quadrature sensitivities solution vectors after a successful return from `CVode`.

Arguments `cvode_mem` (void \*) pointer to the memory previously allocated by `CVodeInit`.  
`tret` (realtype) the time reached by the solver (output).  
`yQS` (N\_Vector \*) array of `Ns` computed sensitivity-dependent quadrature vectors.

Return value The return value `flag` of `CVodeGetQuadSens` is one of:

`CV_SUCCESS` `CVodeGetQuadSens` was successful.  
`CVODE_MEM_NULL` `cvode_mem` was NULL.  
`CV_NO_SENS` Sensitivities were not activated.  
`CV_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.  
`CV_BAD_DKY` `yQS` or one of the `yQS[i]` is NULL.

The function `CVodeGetQuadSensDky` computes the `k`-th derivatives of the interpolating polynomials for the sensitivity-dependent quadrature variables at time `t`. This function is called by `CVodeGetQuadSens` with `k = 0`, but may also be called directly by the user.

#### CVodeGetQuadSensDky

Call `flag = CVodeGetQuadSensDky(cvode_mem, t, k, dkyQS);`

Description The function `CVodeGetQuadSensDky` returns derivatives of the quadrature sensitivities solution vectors after a successful return from `CVode`.

Arguments `cvode_mem` (void \*) pointer to the memory previously allocated by `CVodeInit`.  
`t` (realtype) the time at which information is requested. The time `t` must fall within the interval defined by the last successful step taken by CVODES.  
`k` (int) order of the requested derivative.  
`dkyQS` (N\_Vector \*) array of `Ns` the vector containing the derivatives on output. This vector array must be allocated by the user.

Return value The return value `flag` of `CVodeGetQuadSensDky` is one of:

`CV_SUCCESS` `CVodeGetQuadSensDky` succeeded.  
`CVODE_MEM_NULL` The pointer to `cvode_mem` was NULL.  
`CV_NO_SENS` Sensitivities were not activated.  
`CV_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.  
`CV_BAD_DKY` `dkyQS` or one of the vectors `dkyQS[i]` is NULL.  
`CV_BAD_K` `k` is not in the range 0, 1, ..., `qlast`.  
`CV_BAD_T` The time `t` is not in the allowed range.

Quadrature sensitivity solution vectors can also be extracted separately for each parameter in turn through the functions `CVodeGetQuadSens1` and `CVodeGetQuadSensDky1`, defined as follows:

**CVodeGetQuadSens1**

**Call** `flag = CVodeGetQuadSens1(cvode_mem, &tret, is, yQS);`

**Description** The function `CVodeGetQuadSens1` returns the `is`-th sensitivity of quadratures after a successful return from `CVode`.

**Arguments**

- `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.
- `tret` (`realtype`) the time reached by the solver (output).
- `is` (`int`) specifies which sensitivity vector is to be returned ( $0 \leq is < N_s$ ).
- `yQS` (`N_Vector`) the computed sensitivity-dependent quadrature vector.

**Return value** The return value `flag` of `CVodeGetQuadSens1` is one of:

- `CV_SUCCESS` `CVodeGetQuadSens1` was successful.
- `CVODE_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_SENS` Forward sensitivity analysis was not initialized.
- `CV_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.
- `CV_BAD_IS` The index `is` is not in the allowed range.
- `CV_BAD_DKY` `yQS` is `NULL`.

**CVodeGetQuadSensDky1**

**Call** `flag = CVodeGetQuadSensDky1(cvode_mem, t, k, is, dkyQS);`

**Description** The function `CVodeGetQuadSensDky1` returns the `k`-th derivative of the `is`-th sensitivity solution vector after a successful return from `CVode`.

**Arguments**

- `cvode_mem` (`void *`) pointer to the memory previously allocated by `CVodeInit`.
- `t` (`realtype`) specifies the time at which sensitivity information is requested. The time `t` must fall within the interval defined by the last successful step taken by CVODES.
- `k` (`int`) order of derivative.
- `is` (`int`) specifies the sensitivity derivative vector to be returned ( $0 \leq is < N_s$ ).
- `dkyQS` (`N_Vector`) the vector containing the derivative on output. The space for `dkyQS` must be allocated by the user.

**Return value** The return value `flag` of `CVodeGetQuadSensDky1` is one of:

- `CV_SUCCESS` `CVodeGetQuadDky1` succeeded.
- `CVODE_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_SENS` Forward sensitivity analysis was not initialized.
- `CV_NO_QUADSENS` Quadratures depending on the sensitivities were not activated.
- `CV_BAD_DKY` `dkyQS` is `NULL`.
- `CV_BAD_IS` The index `is` is not in the allowed range.
- `CV_BAD_K` `k` is not in the range  $0, 1, \dots, q_{last}$ .
- `CV_BAD_T` The time `t` is not in the allowed range.

#### 5.4.4 Optional inputs for sensitivity-dependent quadrature integration

CVODES provides the following optional input functions to control the integration of sensitivity-dependent quadrature equations.

**CVodeSetQuadSensErrCon**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeSetQuadSensErrCon(cvode_mem, errconQS)</code>  |
| Description  | The function <code>CVodeSetQuadSensErrCon</code> specifies whether or not the quadrature variables are to be used in the step size control mechanism. If they are, the user must call one of the functions <code>CVodeQuadSensSStolerances</code> , <code>CVodeQuadSensSVtolerances</code> , or <code>CVodeQuadSensEETolerances</code> to specify the integration tolerances for the quadrature variables. |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>errconQS</code> ( <code>boolean_t</code> ) specifies whether sensitivity quadrature variables are to be included ( <code>SUNTRUE</code> ) or not ( <code>SUNFALSE</code> ) in the error control mechanism.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CVODE_MEM_NULL</code> <code>cvode_mem</code> is <code>NULL</code> .<br><code>CV_NO_SENS</code> Sensitivities were not activated.<br><code>CV_NO_QUADSENS</code> Quadratures depending on the sensitivities were not activated.                 |
| Notes        | By default, <code>errconQS</code> is set to <code>SUNFALSE</code> .<br>It is illegal to call <code>CVodeSetQuadSensErrCon</code> before a call to <code>CVodeQuadSensInit</code> .   |



If the quadrature variables are part of the step size control mechanism, one of the following functions must be called to specify the integration tolerances for quadrature variables.

**CVodeQuadSensSStolerances**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeQuadSensSVtolerances(cvode_mem, reltolQS, abstolQS);</code>   |
| Description  | The function <code>CVodeQuadSensSStolerances</code> specifies scalar relative and absolute tolerances.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>reltolQS</code> ( <code>realtype</code> ) is the scalar relative error tolerance.<br><code>abstolQS</code> ( <code>realtype*</code> ) is a pointer to an array containing the <code>Ns</code> scalar absolute error tolerances.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CVODE_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_SENS</code> Sensitivities were not activated.<br><code>CV_NO_QUADSENS</code> Quadratures depending on the sensitivities were not activated.<br><code>CV_ILL_INPUT</code> One of the input tolerances was negative. |

**CVodeQuadSensSVtolerances**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeQuadSensSVtolerances(cvode_mem, reltolQS, abstolQS);</code>   |
| Description  | The function <code>CVodeQuadSensSVtolerances</code> specifies scalar relative and vector absolute tolerances.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>reltolQS</code> ( <code>realtype</code> ) is the scalar relative error tolerance.<br><code>abstolQS</code> ( <code>N_Vector*</code> ) is an array of <code>Ns</code> variables of type <code>N_Vector</code> . The <code>N_Vector</code> <code>abstolS[is]</code> specifies the vector tolerances for <code>is</code> -th quadrature sensitivity. |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional value has been successfully set.<br><code>CV_NO_QUAD</code> Quadrature integration was not initialized.   |

**CVODE\_MEM\_NULL** The `cvode_mem` pointer is `NULL`.  
**CV\_NO\_SENS** Sensitivities were not activated.  
**CV\_NO\_QUADSENS** Quadratures depending on the sensitivities were not activated.  
**CV\_ILL\_INPUT** One of the input tolerances was negative.

#### CVodeQuadSenseEtolerances

**Call** `flag = CVodeQuadSenseEtolerances(cvode_mem);`  
**Description** A call to the function `CVodeQuadSenseEtolerances` specifies that the tolerances for the sensitivity-dependent quadratures should be estimated from those provided for the pure quadrature variables.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
**Return value** The return value `flag` (of type `int`) is one of:  
**CV\_SUCCESS** The optional value has been successfully set.  
**CVODE\_MEM\_NULL** The `cvode_mem` pointer is `NULL`.  
**CV\_NO\_SENS** Sensitivities were not activated.  
**CV\_NO\_QUADSENS** Quadratures depending on the sensitivities were not activated.  
**Notes** When `CVodeQuadSenseEtolerances` is used, before calling `CVode`, integration of pure quadratures must be initialized (see 4.7.1) and tolerances for pure quadratures must be also specified (see 4.7.4).

### 5.4.5 Optional outputs for sensitivity-dependent quadrature integration

CVODES provides the following functions that can be used to obtain solver performance information related to quadrature integration.

#### CVodeGetQuadSensNumRhsEvals

**Call** `flag = CVodeGetQuadSensNumRhsEvals(cvode_mem, &nrhsQSevals);`  
**Description** The function `CVodeGetQuadSensNumRhsEvals` returns the number of calls made to the user's quadrature right-hand side function.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nrhsQSevals` (`long int`) number of calls made to the user's `rhsQS` function.  
**Return value** The return value `flag` (of type `int`) is one of:  
**CV\_SUCCESS** The optional output value has been successfully set.  
**CVODE\_MEM\_NULL** The `cvode_mem` pointer is `NULL`.  
**CV\_NO\_QUADSENS** Sensitivity-dependent quadrature integration has not been initialized.

#### CVodeGetQuadSensNumErrTestFails

**Call** `flag = CVodeGetQuadSensNumErrTestFails(cvode_mem, &nQSetfails);`  
**Description** The function `CVodeGetQuadSensNumErrTestFails` returns the number of local error test failures due to quadrature variables.  
**Arguments** `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`nQSetfails` (`long int`) number of error test failures due to quadrature variables.  
**Return value** The return value `flag` (of type `int`) is one of:  
**CV\_SUCCESS** The optional output value has been successfully set.  
**CVODE\_MEM\_NULL** The `cvode_mem` pointer is `NULL`.  
**CV\_NO\_QUADSENS** Sensitivity-dependent quadrature integration has not been initialized.



**CVodeGetQuadSensErrWeights**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetQuadSensErrWeights(cvode_mem, eQSweight);</code>  |
| Description  | The function <code>CVodeGetQuadSensErrWeights</code> returns the quadrature error weights at the current time.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>eQSweight</code> ( <code>N_Vector *</code> ) array of quadrature error weight vectors at the current time.   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> The optional output value has been successfully set.<br><code>CVODE_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_QUADSENS</code> Sensitivity-dependent quadrature integration has not been initialized. |
| Notes        | The user must allocate memory for <code>eQSweight</code> .<br>If quadratures were not included in the error control mechanism (through a call to <code>CVodeSetQuadSensErrCon</code> with <code>errconQS = SUNTRUE</code> ), then this function does not set the <code>eQSweight</code> array.   |

**CVodeGetQuadSensStats**

|              |  |
|--------------|--|
| Call         | <code>flag = CVodeGetQuadSensStats(cvode_mem, &amp;nrhsQSevals, &amp;nQSetfails);</code>   |
| Description  | The function <code>CVodeGetQuadSensStats</code> returns the CVODES integrator statistics as a group.   |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>nrhsQSevals</code> ( <code>long int</code> ) number of calls to the user's <code>rhsQS</code> function.<br><code>nQSetfails</code> ( <code>long int</code> ) number of error test failures due to quadrature variables.  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> the optional output values have been successfully set.<br><code>CVODE_MEM_NULL</code> the <code>cvode_mem</code> pointer is <code>NULL</code> .<br><code>CV_NO_QUADSENS</code> Sensitivity-dependent quadrature integration has not been initialized. |

### 5.4.6 User-supplied function for sensitivity-dependent quadrature integration

For the integration of sensitivity-dependent quadrature equations, the user must provide a function that defines the right-hand side of those quadrature equations. For the sensitivities of quadratures (2.9) with integrand  $q$ , the appropriate right-hand side functions are given by:  $\bar{q}_i = q_y s_i + q_{p_i}$ . This user function must be of type `CVQuadSensRhsFn` defined as follows:

**CVQuadSensRhsFn**

|            |  |   |  |  |
|------------|--|---|--|--|
| Definition | <pre>typedef int (*CVQuadSensRhsFn)(int Ns, realtype t, N_Vector y,                                 N_Vector yS, N_Vector yQdot,                                 N_Vector *rhssvalQS, void *user_data,                                 N_Vector tmp1, N_Vector tmp2)</pre> |   |  |  |
| Purpose    | This function computes the sensitivity quadrature equation right-hand side for a given value of the independent variable $t$ and state vector $y$ .  |   |  |  |
| Arguments  | <code>Ns</code>  | is the number of sensitivity vectors.   |  |  |
|            | <code>t</code>   | is the current value of the independent variable.   |  |  |
|            | <code>y</code>   | is the current value of the dependent variable vector, $y(t)$ .   |  |  |
|            | <code>yS</code>  | is an array of <code>Ns</code> variables of type <code>N_Vector</code> containing the dependent sensitivity vectors $s_i$ . |  |  |

|              |  |   |
|--------------|--|---|
|              | <code>yQdot</code>   | is the current value of the quadrature right-hand side, $q$ .                   |
|              | <code>rhsvalQS</code>  | array of <code>Ns</code> vectors to contain the right-hand sides.               |
|              | <code>user_data</code>   | is the <code>user_data</code> pointer passed to <code>CVodeSetUserData</code> . |
|              | <code>tmp1</code>  |   |
|              | <code>tmp2</code>  | are <code>N_Vectors</code> which can be used as temporary storage.              |
| Return value | A <code>CVQuadSensRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_QRHS_FAIL</code> is returned).   |   |
| Notes        | <p>Allocation of memory for <code>rhsvalQS</code> is automatically handled within CVODES.</p> <p>Here <code>y</code> is of type <code>N_Vector</code> and <code>yS</code> is a pointer to an array containing <code>Ns</code> vectors of type <code>N_Vector</code>. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each <code>NVECTOR</code> implementation). For the sake of computational efficiency, the vector functions in the two <code>NVECTOR</code> implementations provided with CVODES do not perform any consistency checks with respect to their <code>N_Vector</code> arguments (see §7.1 and §7.2).</p> <p>There are two situations in which recovery is not possible even if <code>CVQuadSensRhsFn</code> function returns a recoverable error flag. One is when this occurs at the very first call to the <code>CVQuadSensRhsFn</code> (in which case CVODES returns <code>CV_FIRST_QSRHSFUNC_ERR</code>). The other is when a recoverable error is reported by <code>CVQuadSensRhsFn</code> after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODES returns <code>CV_UNREC_QSRHSFUNC_ERR</code>).</p> |   |

## 5.5 Note on using partial error control

For some problems, when sensitivities are excluded from the error control test, the behavior of CVODES may appear at first glance to be erroneous. One would expect that, in such cases, the sensitivity variables would not influence in any way the step size selection. A comparison of the solver diagnostics reported for `cvsdex` and the second run of the `cvsfwddex` example in [35] indicates that this may not always be the case.

The short explanation of this behavior is that the step size selection implemented by the error control mechanism in CVODES is based on the magnitude of the correction calculated by the nonlinear solver. As mentioned in §5.2.1, even with partial error control selected (in the call to `CVodeSetSensErrCon`), the sensitivity variables are included in the convergence tests of the nonlinear solver.

When using the simultaneous corrector method (§2.6), the nonlinear system that is solved at each step involves both the state and sensitivity equations. In this case, it is easy to see how the sensitivity variables may affect the convergence rate of the nonlinear solver and therefore the step size selection. The case of the staggered corrector approach is more subtle. After all, in this case (`ism` = `CV_STAGGERED` or `CV_STAGGERED1` in the call to `CVodeSensInit/CVodeSensInit1`), the sensitivity variables at a given step are computed only once the solver for the nonlinear state equations has converged. However, if the nonlinear system corresponding to the sensitivity equations has convergence problems, CVODES will attempt to improve the initial guess by reducing the step size in order to provide a better prediction of the sensitivity variables. Moreover, even if there are no convergence failures in the solution of the sensitivity system, CVODES may trigger a call to the linear solver's setup routine which typically involves reevaluation of Jacobian information (Jacobian approximation in the case of `CVDENSE` and `CVBAND`, or preconditioner data in the case of the Krylov solvers). The new Jacobian information will be used by subsequent calls to the nonlinear solver for the state equations and, in this way, potentially affect the step size selection.

When using the simultaneous corrector method it is not possible to decide whether nonlinear solver convergence failures or calls to the linear solver setup routine have been triggered by convergence problems due to the state or the sensitivity equations. When using one of the staggered corrector methods however, these situations can be identified by carefully monitoring the diagnostic information

provided through optional outputs. If there are no convergence failures in the sensitivity nonlinear solver, and none of the calls to the linear solver setup routine were made by the sensitivity nonlinear solver, then the step size selection is not affected by the sensitivity variables.

Finally, the user must be warned that the effect of appending sensitivity equations to a given system of ODEs on the step size selection (through the mechanisms described above) is problem-dependent and can therefore lead to either an increase or decrease of the total number of steps that CVODES takes to complete the simulation. At first glance, one would expect that the impact of the sensitivity variables, if any, would be in the direction of increasing the step size and therefore reducing the total number of steps. The argument for this is that the presence of the sensitivity variables in the convergence test of the nonlinear solver can only lead to additional iterations (and therefore a smaller final iteration error), or to additional calls to the linear solver setup routine (and therefore more up-to-date Jacobian information), both of which will lead to larger steps being taken by CVODES. However, this is true only locally. Overall, a larger integration step taken at a given time may lead to step size reductions at later times, due to either nonlinear solver convergence failures or error test failures.



## Chapter 6

# Using CVODES for Adjoint Sensitivity Analysis

This chapter describes the use of CVODES to compute sensitivities of derived functions using adjoint sensitivity analysis. As mentioned before, the adjoint sensitivity module of CVODES provides the infrastructure for integrating backward in time any system of ODEs that depends on the solution of the original IVP, by providing various interfaces to the main CVODES integrator, as well as several supporting user-callable functions. For this reason, in the following sections we refer to the *backward problem* and not to the *adjoint problem* when discussing details relevant to the ODEs that are integrated backward in time. The backward problem can be the adjoint problem (2.19) or (2.22), and can be augmented with some quadrature differential equations.

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

We begin with a brief overview, in the form of a skeleton user program. Following that are detailed descriptions of the interface to the various user-callable functions and of the user-supplied functions that were not already described in Chapter 4.

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

The following is a skeleton of the user's main program as an application of CVODES. The user program is to have these steps in the order indicated, unless otherwise noted. For the sake of brevity, we defer many of the details to the later sections. As in §4.4, most steps are independent of the NVECTOR implementation used; where this is not the case, refer to Chapter 7 for specifics. Steps that are unchanged from the skeleton programs presented in §4.4, §5.1, and §5.4, are grayed out.

1. Include necessary header files

The `cvodes.h` header file also defines additional types, constants, and function prototypes for the adjoint sensitivity module user-callable functions. In addition, the main program should include an NVECTOR implementation header file (for the particular implementation used), and, if Newton iteration was selected, the main header file of the desired linear solver module.

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

#### Forward problem

3. Set problem dimensions etc. for the forward problem

4. Set initial conditions for the forward problem

5. Create CVODES object for the forward problem

6. **Initial CVODES for the forward problem**
7. **Specify integration tolerances for forward problem**
8. **Set optional inputs for the forward problem**
9. **Create matrix object for the forward problem**
10. **Create linear solver object for the forward problem**
11. **Set linear solver optional inputs for the forward problem**
12. **Attach linear solver module for the forward problem**
13. **Initialize quadrature problem or problems for forward problems, using `CVodeQuadInit` and/or `CVodeQuadSensInit`.**
14. **Initialize forward sensitivity problem**
15. **Specify rootfinding**
16. **Allocate space for the adjoint computation**  
 Call `CVodeAdjInit()` to allocate memory for the combined forward-backward problem (see §6.2.1 for details). This call requires `Nd`, the number of steps between two consecutive checkpoints. `CVodeAdjInit` also specifies the type of interpolation used (see §2.7.1).

**17. Integrate forward problem**

Call `CVodeF`, a wrapper for the CVODES main integration function `CVode`, either in `CV_NORMAL` mode to the time `tout` or in `CV_ONE_STEP` mode inside a loop (if intermediate solutions of the forward problem are desired (see §6.2.2)). The final value of `tret` is then the maximum allowable value for the endpoint  $T$  of the backward problem.

### Backward problem(s)

18. **Set problem dimensions etc. for the backward problem**  
 This generally includes the backward problem vector length `NB`, and possibly the local vector length `NBlocal`.
19. **Set initial values for the backward problem**  
 Set the endpoint time `tB0` =  $T$ , and set the corresponding vector `yB0` at which the backward problem starts.
20. **Create the backward problem**  
 Call `CVodeCreateB`, a wrapper for `CVodeCreate`, to create the CVODES memory block for the new backward problem. Unlike `CVodeCreate`, the function `CVodeCreateB` does not return a pointer to the newly created memory block (see §6.2.3). Instead, this pointer is attached to the internal adjoint memory block (created by `CVodeAdjInit`) and returns an identifier called `which` that the user must later specify in any actions on the newly created backward problem.
21. **Allocate memory for the backward problem**  
 Call `CVodeInitB` (or `CVodeInitBS`, when the backward problem depends on the forward sensitivities). The two functions are actually wrappers for `CVodeInit` and allocate internal memory, specify problem data, and initialize CVODES at `tB0` for the backward problem (see §6.2.3).
22. **Specify integration tolerances for backward problem**

Call `CVodeSStolerancesB(...)` or `CVodeSVtolerancesB(...)` to specify a scalar relative tolerance and scalar absolute tolerance or scalar relative tolerance and a vector of absolute tolerances, respectively. The functions are wrappers for `CVodeSStolerances` and `CVodeSVtolerances`, but they require an extra argument `which`, the identifier of the backward problem returned by `CVodeCreateB`. See §6.2.4 for more information.

### 23. Set optional inputs for the backward problem

Call `CVodeSet*B` functions to change from their default values any optional inputs that control the behavior of CVODES. Unlike their counterparts for the forward problem, these functions take an extra argument `which`, the identifier of the backward problem returned by `CVodeCreateB` (see §6.2.8).

### 24. Create matrix object for the backward problem

If a direct linear solver is to be used within a Newton iteration then a template Jacobian matrix must be created by using the appropriate functions defined by the particular SUNMATRIX implementation.

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

Note also that it is not required to use the same matrix type for both the forward and the backward problems.

### 25. Create linear solver object for the backward problem

Create the linear solver object for the backward problem by using the appropriate functions defined by the particular SUNLINSOL implementation desired.

Note that it is not required to use the same linear solver module for both the forward and the backward problems; for example, the forward problem could be solved with the CVDLS linear solver module and the backward problem with CVSPILS linear solver module.

### 26. Set linear solver interface optional inputs for the backward problem

Call `CVDlsSet*B` or `CVSpilsSet*B` functions to change optional inputs specific to that linear solver interface. See §6.2.8 for details.

### 27. Initialize quadrature calculation

If additional quadrature equations must be evaluated, call `CVodeQuadInitB` or `CVodeQuadInitBS` (if quadrature depends also on the forward sensitivities) as shown in §6.2.10.1. These functions are wrappers around `CVodeQuadInit` and can be used to initialize and allocate memory for quadrature integration. Optionally, call `CVodeSetQuad*B` functions to change from their default values optional inputs that control the integration of quadratures during the backward phase.

### 28. Integrate backward problem

Call `CVodeB`, a second wrapper around the CVODES main integration function `CVode`, to integrate the backward problem from `tb0` (see §6.2.6). This function can be called either in `CV_NORMAL` or `CV_ONE_STEP` mode. Typically, `CVodeB` will be called in `CV_NORMAL` mode with an end time equal to the initial time  $t_0$  of the forward problem.

### 29. Extract quadrature variables

If applicable, call `CVodeGetQuadB`, a wrapper around `CVodeGetQuad`, to extract the values of the quadrature variables at the time returned by the last call to `CVodeB`. See §6.2.10.2.

### 30. Deallocate memory

Upon completion of the backward integration, call all necessary deallocation functions. These include appropriate destructors for the vectors `y` and `yB`, a call to `CVodeFree` to free the CVODES

memory block for the forward problem. If one or more additional Adjoint Sensitivity Analyses are to be done for this problem, a call to `CVodeAdjFree` (see §6.2.1) may be made to free and deallocate memory allocated for the backward problems, followed by a call to `CVodeAdjInit`.

### 31. Free linear solver and matrix memory for the backward problem

### 32. Finalize MPI, if used

The above user interface to the adjoint sensitivity module in CVODES was motivated by the desire to keep it as close as possible in look and feel to the one for ODE IVP integration. Note that if steps (18)-(29) are not present, a program with the above structure will have the same functionality as one described in §4.4 for integration of ODEs, albeit with some overhead due to the checkpointing scheme.

If there are multiple backward problems associated with the same forward problem, repeat steps (18)-(29) above for each successive backward problem. In the process, each call to `CVodeCreateB` creates a new value of the identifier `which`.

## 6.2 User-callable functions for adjoint sensitivity analysis

### 6.2.1 Adjoint sensitivity allocation and deallocation functions

After the setup phase for the forward problem, but before the call to `CVodeF`, memory for the combined forward-backward problem must be allocated by a call to the function `CVodeAdjInit`. The form of the call to this function is

`CVodeAdjInit`

Call `flag = CVodeAdjInit(cvode_mem, Nd, interpType);`

Description The function `CVodeAdjInit` updates CVODES memory block by allocating the internal memory needed for backward integration. Space is allocated for the  $N_d = N_d$  interpolation data points, and a linked list of checkpoints is initialized.

Arguments `cvode_mem` (`void *`) is the pointer to the CVODES memory block returned by a previous call to `CVodeCreate`.

`Nd` (`long int`) is the number of integration steps between two consecutive checkpoints.

`interpType` (`int`) specifies the type of interpolation used and can be `CV_POLYNOMIAL` or `CV_HERMITE`, indicating variable-degree polynomial and cubic Hermite interpolation, respectively (see §2.7.1).

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

`CV_SUCCESS` `CVodeAdjInit` was successful.

`CV_MEM_FAIL` A memory allocation request has failed.

`CV_MEM_NULL` `cvode_mem` was NULL.

`CV_ILL_INPUT` One of the parameters was invalid: `Nd` was not positive or `interpType` is not one of the `CV_POLYNOMIAL` or `CV_HERMITE`.

Notes The user must set `Nd` so that all data needed for interpolation of the forward problem solution between two checkpoints fits in memory. `CVodeAdjInit` attempts to allocate space for  $(2N_d+3)$  variables of type `N_Vector`.

If an error occurred, `CVodeAdjInit` also sends a message to the error handler function.

`CVodeAdjReInit`

Call `flag = CVodeAdjReInit(cvode_mem);`



|              |   |
|--------------|---|
| Description  | The function <code>CVodeAdjReInit</code> reinitializes the CVODES memory block for ASA, assuming that the number of steps between check points and the type of interpolation remain unchanged.  |
| Arguments    | <code>cvode_mem</code> ( <code>void *</code> ) is the pointer to the CVODES memory block returned by a previous call to <code>CVodeCreate</code> .  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:<br><code>CV_SUCCESS</code> <code>CVodeAdjReInit</code> was successful.<br><code>CV_MEM_NULL</code> <code>cvode_mem</code> was <code>NULL</code> .<br><code>CV_NO_ADJ</code> The function <code>CVodeAdjInit</code> was not previously called.   |
| Notes        | The list of check points (and associated memory) is deleted.<br><br>The list of backward problems is kept. However, new backward problems can be added to this list by calling <code>CVodeCreateB</code> . If a new list of backward problems is also needed, then free the adjoint memory (by calling <code>CVodeAdjFree</code> ) and reinitialize ASA with <code>CVodeAdjInit</code> .<br><br>The CVODES memory for the forward and backward problems can be reinitialized separately by calling <code>CVodeReInit</code> and <code>CVodeReInitB</code> , respectively. |

#### CVodeAdjFree

|              |  |
|--------------|--|
| Call         | <code>CVodeAdjFree(cvode_mem);</code>  |
| Description  | The function <code>CVodeAdjFree</code> frees the memory related to backward integration allocated by a previous call to <code>CVodeAdjInit</code> .  |
| Arguments    | The only argument is the CVODES memory block pointer returned by a previous call to <code>CVodeCreate</code> .   |
| Return value | The function <code>CVodeAdjFree</code> has no return value.  |
| Notes        | This function frees all memory allocated by <code>CVodeAdjInit</code> . This includes workspace memory, the linked list of checkpoints, memory for the interpolation data, as well as the CVODES memory for the backward integration phase. Unless one or more further calls to <code>CVodeAdjInit</code> are to be made, <code>CVodeAdjFree</code> should not be called by the user, as it is invoked automatically by <code>CVodeFree</code> . |

### 6.2.2 Forward integration function

The function `CVodeF` is very similar to the CVODES function `CVode` (see §4.5.5) in that it integrates the solution of the forward problem and returns the solution in `y`. At the same time, however, `CVodeF` stores checkpoint data every `Nd` integration steps. `CVodeF` can be called repeatedly by the user. Note that `CVodeF` is used only for the forward integration pass within an Adjoint Sensitivity Analysis. It is not for use in Forward Sensitivity Analysis; for that, see Chapter 5. The call to this function has the form

#### CVodeF

|             |  |
|-------------|--|
| Call        | <code>flag = CVodeF(cvode_mem, tout, yret, &amp;tret, itask, &amp;ncheck);</code>  |
| Description | The function <code>CVodeF</code> integrates the forward problem over an interval in $t$ and saves checkpointing data.  |
| Arguments   | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>tout</code> ( <code>realtype</code> ) the next time at which a computed solution is desired.<br><code>yret</code> ( <code>N_Vector</code> ) the computed solution vector $y$ .<br><code>tret</code> ( <code>realtype</code> ) the time reached by the solver (output). |

|                         |  |
|-------------------------|--|
| <b>itask</b>            | ( <b>int</b> ) a flag indicating the job of the solver for the next step. The <b>CV_NORMAL</b> task is to have the solver take internal steps until it has reached or just passed the user-specified <b>tout</b> parameter. The solver then interpolates in order to return an approximate value of $y(\mathbf{tout})$ . The <b>CV_ONE_STEP</b> option tells the solver to just take one internal step and return the solution at the point reached by that step.  |
| <b>ncheck</b>           | ( <b>int</b> ) the number of (internal) checkpoints stored so far.   |
| <b>Return value</b>     | On return, <b>CVodeF</b> returns the vector <b>yret</b> and a corresponding independent variable value $t = \mathbf{tret}$ , such that <b>yret</b> is the computed value of $y(t)$ . Additionally, it returns in <b>ncheck</b> the number of internal checkpoints saved; the total number of checkpoint intervals is <b>ncheck</b> +1. The return value <b>flag</b> (of type <b>int</b> ) will be one of the following. For more details see §4.5.5.   |
| <b>CV_SUCCESS</b>       | <b>CVodeF</b> succeeded.   |
| <b>CV_TSTOP_RETURN</b>  | <b>CVodeF</b> succeeded by reaching the optional stopping point.   |
| <b>CV_ROOT_RETURN</b>   | <b>CVodeF</b> succeeded and found one or more roots. In this case, <b>tret</b> is the location of the root. If <b>nrtfn</b> > 1, call <b>CVodeGetRootInfo</b> to see which $g_i$ were found to have a root.  |
| <b>CV_NO_MALLOC</b>     | The function <b>CVodeInit</b> has not been previously called.  |
| <b>CV_ILL_INPUT</b>     | One of the inputs to <b>CVodeF</b> is illegal.   |
| <b>CV_TOO_MUCH_WORK</b> | The solver took <b>mxstep</b> internal steps but could not reach <b>tout</b> .   |
| <b>CV_TOO_MUCH_ACC</b>  | The solver could not satisfy the accuracy demanded by the user for some internal step.   |
| <b>CV_ERR_FAILURE</b>   | Error test failures occurred too many times during one internal time step or occurred with $ h  = h_{min}$ .   |
| <b>CV_CONV_FAILURE</b>  | Convergence test failures occurred too many times during one internal time step or occurred with $ h  = h_{min}$ .   |
| <b>CV_LSETUP_FAIL</b>   | The linear solver's setup function failed in an unrecoverable manner.  |
| <b>CV_LSOLVE_FAIL</b>   | The linear solver's solve function failed in an unrecoverable manner.  |
| <b>CV_NO_ADJ</b>        | The function <b>CVodeAdjInit</b> has not been previously called.   |
| <b>CV_MEM_FAIL</b>      | A memory allocation request has failed (in an attempt to allocate space for a new checkpoint).   |
| <b>Notes</b>            | <p>All failure return values are negative and therefore a test <b>flag</b> &lt; 0 will trap all <b>CVodeF</b> failures.</p> <p>At this time, <b>CVodeF</b> stores checkpoint information in memory only. Future versions will provide for a safeguard option of dumping checkpoint data into a temporary file as needed. The data stored at each checkpoint is basically a snapshot of the CVODES internal memory block and contains enough information to restart the integration from that time and to proceed with the same step size and method order sequence as during the forward integration.</p> <p>In addition, <b>CVodeF</b> also stores interpolation data between consecutive checkpoints so that, at the end of this first forward integration phase, interpolation information is already available from the last checkpoint forward. In particular, if no checkpoints were necessary, there is no need for the second forward integration phase.</p> <p>It is illegal to change the integration tolerances between consecutive calls to <b>CVodeF</b>, as this information is not captured in the checkpoint data.</p> |



### 6.2.3 Backward problem initialization functions

The functions **CVodeCreateB** and **CVodeInitB** (or **CVodeInitBS**) must be called in the order listed. They instantiate a CVODES solver object, provide problem and solution specifications, and allocate internal memory for the backward problem.

**CVodeCreateB**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeCreateB(cvode_mem, lmmB, iterB, &amp;which);</code>   |
| Description  | The function <code>CVodeCreateB</code> instantiates a CVODES solver object and specifies the solution method for the backward problem.  |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>lmmB</code> (int) specifies the linear multistep method and may be one of two possible values: <code>CV_ADAMS</code> or <code>CV_BDF</code>.</p> <p><code>iterB</code> (int) specifies the type of nonlinear solver iteration and may be either <code>CV_NEWTON</code> or <code>CV_FUNCTIONAL</code>.</p> <p><code>which</code> (int) contains the identifier assigned by CVODES for the newly created backward problem. Any call to <code>CVode*B</code> functions requires such an identifier.</p> |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeCreateB</code> was successful.</p> <p><code>CV_MEM_NULL</code> <code>cvode_mem</code> was NULL.</p> <p><code>CV_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.</p> <p><code>CV_MEM_FAIL</code> A memory allocation request has failed.</p>  |

There are two initialization functions for the backward problem – one for the case when the backward problem does not depend on the forward sensitivities, and one for the case when it does. These two functions are described next.

The function `CVodeInitB` initializes the backward problem when it does not depend on the forward sensitivities. It is essentially a wrapper for `CVodeInit` with some particularization for backward integration, as described below.

**CVodeInitB**

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeInitB(cvode_mem, which, rhsB, tB0, yB0);</code>   |
| Description  | The function <code>CVodeInitB</code> provides problem specification, allocates internal memory, and initializes the backward problem.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>which</code> (int) represents the identifier of the backward problem.</p> <p><code>rhsB</code> (<code>CVRhsFnB</code>) is the C function which computes <math>fB</math>, the right-hand side of the backward ODE problem. This function has the form <code>rhsB(t, y, yB, yBdot, user_dataB)</code> (for full details see §6.3.1).</p> <p><code>tB0</code> (<code>realtype</code>) specifies the endpoint <math>T</math> where final conditions are provided for the backward problem, normally equal to the endpoint of the forward integration.</p> <p><code>yB0</code> (<code>N_Vector</code>) is the initial value (at <math>t = tB0</math>) of the backward solution.</p> |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeInitB</code> was successful.</p> <p><code>CV_NO_MALLOC</code> The function <code>CVodeInit</code> has not been previously called.</p> <p><code>CV_MEM_NULL</code> <code>cvode_mem</code> was NULL.</p> <p><code>CV_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.</p> <p><code>CV_BAD_TB0</code> The final time <code>tB0</code> was outside the interval over which the forward problem was solved.</p> <p><code>CV_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier, or either <code>yB0</code> or <code>rhsB</code> was NULL.</p>                                      |
| Notes        | The memory allocated by <code>CVodeInitB</code> is deallocated by the function <code>CVodeAdjFree</code> .  |

For the case when backward problem also depends on the forward sensitivities, user must call `CVodeInitBS` instead of `CVodeInitB`. Only the third argument of each function differs between these two functions.

**CVodeInitBS**

**Call** `flag = CVodeInitBS(cvode_mem, which, rhsBS, tB0, yB0);`

**Description** The function `CVodeInitBS` provides problem specification, allocates internal memory, and initializes the backward problem.

**Arguments**

- `cvode_mem` (`void *`) pointer to the CVODES memory block returned by `CVodeCreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `rhsBS` (`CVRhsFnBS`) is the C function which computes  $fB$ , the right-hand side of the backward ODE problem. This function has the form `rhsBS(t, y, yS, yB, yBdot, user_dataB)` (for full details see §6.3.2).
- `tB0` (`realtype`) specifies the endpoint  $T$  where final conditions are provided for the backward problem.
- `yB0` (`N_Vector`) is the initial value (at  $t = tB0$ ) of the backward solution.

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

- `CV_SUCCESS` The call to `CVodeInitB` was successful.
- `CV_NO_MALLOC` The function `CVodeInit` has not been previously called.
- `CV_MEM_NULL` `cvode_mem` was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_BAD_TB0` The final time `tB0` was outside the interval over which the forward problem was solved.
- `CV_ILL_INPUT` The parameter `which` represented an invalid identifier, either `yB0` or `rhsBS` was `NULL`, or sensitivities were not active during the forward integration.

**Notes** The memory allocated by `CVodeInitBS` is deallocated by the function `CVodeAdjFree`.

The function `CVodeReInitB` reinitializes CVODES for the solution of a series of backward problems, each identified by a value of the parameter `which`. `CVodeReInitB` is essentially a wrapper for `CVodeReInit`, and so all details given for `CVodeReInit` in §4.5.9 apply here. Also note that `CVodeReInitB` can be called to reinitialize the backward problem even it has been initialized with the sensitivity-dependent version `CVodeInitBS`. Before calling `CVodeReInitB` for a new backward problem, call any desired solution extraction functions `CVodeGet**` associated with the previous backward problem. The call to the `CVodeReInitB` function has the form

**CVodeReInitB**

**Call** `flag = CVodeReInitB(cvode_mem, which, tB0, yB0)`

**Description** The function `CVodeReInitB` reinitializes a CVODES backward problem.

**Arguments**

- `cvode_mem` (`void *`) pointer to CVODES memory block returned by `CVodeCreate`.
- `which` (`int`) represents the identifier of the backward problem.
- `tB0` (`realtype`) specifies the endpoint  $T$  where final conditions are provided for the backward problem.
- `yB0` (`N_Vector`) is the initial value (at  $t = tB0$ ) of the backward solution.

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

- `CV_SUCCESS` The call to `CVodeReInitB` was successful.
- `CV_NO_MALLOC` The function `CVodeInit` has not been previously called.
- `CV_MEM_NULL` The `cvode_mem` memory block pointer was `NULL`.
- `CV_NO_ADJ` The function `CVodeAdjInit` has not been previously called.
- `CV_BAD_TB0` The final time `tB0` is outside the interval over which the forward problem was solved.
- `CV_ILL_INPUT` The parameter `which` represented an invalid identifier, or `yB0` was `NULL`.

### 6.2.4 Tolerance specification functions for backward problem

One of the following two functions must be called to specify the integration tolerances for the backward problem. Note that this call must be made after the call to `CVodeInitB` or `CVodeInitBS`.

#### `CVodeSStolerancesB`

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSStolerancesB(cvode_mem, which, reltolB, abstolB);</code>   |
| Description  | The function <code>CVodeSStolerancesB</code> specifies scalar relative and absolute tolerances.   |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>which</code> (int) represents the identifier of the backward problem.</p> <p><code>reltolB</code> (realtype) is the scalar relative error tolerance.</p> <p><code>abstolB</code> (realtype) is the scalar absolute error tolerance.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeSStolerancesB</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODES memory block was not initialized through a previous call to <code>CVodeCreate</code>.</p> <p><code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called.</p> <p><code>CV_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.</p> <p><code>CV_ILL_INPUT</code> One of the input tolerances was negative.</p> |

#### `CVodeSVtolerancesB`

|              |   |
|--------------|---|
| Call         | <code>flag = CVodeSVtolerancesB(cvode_mem, which, reltol, abstol);</code>   |
| Description  | The function <code>CVodeSVtolerancesB</code> specifies scalar relative tolerance and vector absolute tolerances.  |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>which</code> (int) represents the identifier of the backward problem.</p> <p><code>reltol</code> (realtype) is the scalar relative error tolerance.</p> <p><code>abstol</code> (N_Vector) is the vector of absolute error tolerances.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) will be one of the following:</p> <p><code>CV_SUCCESS</code> The call to <code>CVodeSVtolerancesB</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODES memory block was not initialized through a previous call to <code>CVodeCreate</code>.</p> <p><code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called.</p> <p><code>CV_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.</p> <p><code>CV_ILL_INPUT</code> The relative error tolerance was negative or the absolute tolerance had a negative component.</p> |
| Notes        | This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the state vector $y$ .   |

### 6.2.5 Linear solver initialization functions for backward problem

All CVODES linear solver modules available for forward problems are available for the backward problem. They should be created as for the forward problem then attached to the memory structure for the backward problem using one of the following functions.

**CVDlsSetLinearSolverB**

|              |  |
|--------------|--|
| Call         | <code>flag = CVDlsSetLinearSolverB(cvode_mem, which, LS, A);</code>  |
| Description  | <p>The function <code>CVDlsSetLinearSolverB</code> attaches a direct SUNLINSOL object <code>LS</code> and corresponding template Jacobian SUNMATRIX object <code>A</code> to CVODES, initializing the CVDLS direct linear solver interface for solution of the backward problem.</p> <p>The user's main program must include the <code>cvodes_direct.h</code> header file.</p>   |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the IDAS memory block.</p> <p><code>which</code> (<code>int</code>) represents the identifier of the backward problem returned by <code>CVodeCreateB</code>.</p> <p><code>LS</code> (<code>SUNLinearSolver</code>) SUNLINSOL object to use for solving Newton linear systems for the backward problem.</p> <p><code>A</code> (<code>SUNMatrix</code>) SUNMATRIX object for used as a template for the Jacobian for the backward problem (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 current NVECTOR module.</p> <p><code>CVDLS_MEM_FAIL</code> A memory allocation request failed.</p> <p><code>CVDLS_NO_ADJ</code> The function <code>CVAdjInit</code> has not been previously called.</p> <p><code>CVDLS_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier.</p> |
| Notes        | <p>The CVDLS linear solver 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 9.</p>   |

**CVSpilsSetLinearSolverB**

|              |  |
|--------------|--|
| Call         | <code>flag = CVSpilsSetLinearSolverB(ida_mem, which, LS);</code>   |
| Description  | <p>The function <code>CVSpilsSetLinearSolver</code> attaches an iterative SUNLINSOL object <code>LS</code> to CVODES, initializing the CVSPILS scaled, preconditioned, iterative linear solver interface to use for the backward problem.</p> <p>The user's main program must include the <code>cvs_spils.h</code> header file.</p>  |
| Arguments    | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block.</p> <p><code>which</code> (<code>int</code>) represents the identifier of the backward problem returned by <code>CVodeCreateB</code>.</p> <p><code>LS</code> (<code>SUNLinearSolver</code>) SUNLINSOL object to use for solving Newton linear systems for the backward problem.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CVSPILS_SUCCESS</code> The CVSPILS initialization was successful.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</p> <p><code>CVSPILS_ILL_INPUT</code> The CVSPILS solver is not compatible with the current NVECTOR module.</p> <p><code>CVSPILS_MEM_FAIL</code> A memory allocation request failed.</p> <p><code>CVSPILS_NO_ADJ</code> The function <code>CVAdjInit</code> has not been previously called.</p> <p><code>CVSPILS_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier.</p> |

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 9.

### 6.2.6 Backward integration function

The function `CVodeB` performs the integration of the backward problem. It is essentially a wrapper for the CVODES main integration function `CVode` and, in the case in which checkpoints were needed, it evolves the solution of the backward problem through a sequence of forward-backward integration pairs between consecutive checkpoints. The first run of each pair integrates the original IVP forward in time and stores interpolation data; the second run integrates the backward problem backward in time and performs the required interpolation to provide the solution of the IVP to the backward problem.

The function `CVodeB` does not return the solution  $y_B$  itself. To obtain that, call the function `CVodeGetB`, which is also described below.

The `CVodeB` function does not support rootfinding, unlike `CVodeF`, which supports the finding of roots of functions of  $(t, y)$ . If rootfinding was performed by `CVodeF`, then for the sake of efficiency, it should be disabled for `CVodeB` by first calling `CVodeRootInit` with `nrtfn = 0`.

The call to `CVodeB` has the form

#### `CVodeB`

Call      `flag = CVodeB(cvode_mem, tBout, itaskB);`

Description      The function `CVodeB` integrates the backward ODE problem.

Arguments      `cvode_mem` (void \*) pointer to the CVODES memory returned by `CVodeCreate`.  
                  `tBout` (realtype) the next time at which a computed solution is desired.  
                  `itaskB` (int) a flag indicating the job of the solver for the next step. The `CV_NORMAL` task is to have the solver take internal steps until it has reached or just passed the user-specified value `tBout`. The solver then interpolates in order to return an approximate value of  $y_B(tBout)$ . The `CV_ONE_STEP` option tells the solver to take just one internal step in the direction of `tBout` and return.

Return value      The return value `flag` (of type `int`) will be one of the following. For more details see §4.5.5.


|                               |  |
|-------------------------------|--|
| <code>CV_SUCCESS</code>       | <code>CVodeB</code> succeeded.   |
| <code>CV_MEM_NULL</code>      | <code>cvode_mem</code> was NULL.   |
| <code>CV_NO_ADJ</code>        | The function <code>CVodeAdjInit</code> has not been previously called.                                     |
| <code>CV_NO_BCK</code>        | No backward problem has been added to the list of backward problems by a call to <code>CVodeCreateB</code> |
| <code>CV_NO_FWD</code>        | The function <code>CVodeF</code> has not been previously called.   |
| <code>CV_ILL_INPUT</code>     | One of the inputs to <code>CVodeB</code> is illegal.   |
| <code>CV_BAD_ITASK</code>     | The <code>itaskB</code> argument has an illegal value.   |
| <code>CV_TOO_MUCH_WORK</code> | The solver took <code>mxstep</code> internal steps but could not reach <code>tBout</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>   | Error test failures occurred too many times during one internal time step.                                 |
| <code>CV_CONV_FAILURE</code>  | Convergence test failures occurred too many times during one internal time step.                           |
| <code>CV_LSETUP_FAIL</code>   | The linear solver's setup function failed in an unrecoverable manner.                                      |
| <code>CV_SOLVE_FAIL</code>    | The linear solver's solve function failed in an unrecoverable manner.                                      |



|       |  |  |
|-------|--|--|
|       | CV_BCKMEM_NULL   | The solver memory for the backward problem was not created with a call to <code>CVodeCreateB</code> .                              |
|       | CV_BAD_TBOUT   | The desired output time <code>tBout</code> is outside the interval over which the forward problem was solved.                      |
|       | CV_REIFWD_FAIL   | Reinitialization of the forward problem failed at the first checkpoint (corresponding to the initial time of the forward problem). |
|       | CV_FWD_FAIL  | An error occurred during the integration of the forward problem.   |
| Notes | All failure return values are negative and therefore a test <code>flag &lt; 0</code> will trap all <code>CVodeB</code> failures.   |  |
|       | In the case of multiple checkpoints and multiple backward problems, a given call to <code>CVodeB</code> in <code>CV_ONE_STEP</code> mode may not advance every problem one step, depending on the relative locations of the current times reached. But repeated calls will eventually advance all problems to <code>tBout</code> . |  |

To obtain the solution `yB` to the backward problem, call the function `CVodeGetB` as follows:

#### CVodeGetB

|   |  |  |
|---|--|--|
| Call  | <code>flag = CVodeGetB(cvode_mem, which, &amp;tret, yB);</code>  |  |
| Description   | The function <code>CVodeGetB</code> provides the solution <code>yB</code> of the backward ODE problem.   |  |
| Arguments   | <code>cvode_mem</code> (void *) pointer to the CVODES memory returned by <code>CVodeCreate</code> .<br><code>which</code> (int) the identifier of the backward problem.<br><code>tret</code> (realtype) the time reached by the solver (output).<br><code>yB</code> (N_Vector) the backward solution at time <code>tret</code> . |  |
| Return value  | The return value <code>flag</code> (of type <code>int</code> ) will be one of the following.   |  |
|   | CV_SUCCESS <code>CVodeGetB</code> was successful.  |  |
|   | CV_MEM_NULL <code>cvode_mem</code> is NULL.  |  |
|   | CV_NO_ADJ    The function <code>CVodeAdjInit</code> has not been previously called.  |  |
|   | CV_ILL_INPUT   The parameter <code>which</code> is an invalid identifier.  |  |
|  Notes | The user must allocate space for <code>yB</code> .   |  |

### 6.2.7 Adjoint sensitivity optional input

At any time during the integration of the forward problem, the user can disable the checkpointing of the forward sensitivities by calling the following function:

#### CVodeAdjSetNoSensi

|              |  |  |
|--------------|--|--|
| Call         | <code>flag = CVodeAdjSetNoSensi(cvode_mem);</code>   |  |
| Description  | The function <code>CVodeAdjSetNoSensi</code> instructs <code>CVodeF</code> not to save checkpointing data for forward sensitivities anymore. |  |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.  |  |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of:  |  |
|              | CV_SUCCESS    The call to <code>CVodeCreateB</code> was successful.  |  |
|              | CV_MEM_NULL <code>cvode_mem</code> was NULL.   |  |
|              | CV_NO_ADJ    The function <code>CVodeAdjInit</code> has not been previously called.  |  |



## 6.2.8 Optional input functions for the backward problem

### 6.2.8.1 Main solver optional input functions

The adjoint module in CVODES provides wrappers for most of the optional input functions defined in §4.5.6.1. The only difference is that the user must specify the identifier `which` of the backward problem within the list managed by CVODES.

The optional input functions defined for the backward problem are:

```
flag = CNodeSetUserDataB(cnode_mem, which, user_dataB);
flag = CNodeSetIterTypeB(cnode_mem, which, iterB);
flag = CNodeSetMaxOrdB(cnode_mem, which, maxordB);
flag = CNodeSetMaxNumStepsB(cnode_mem, which, mxstepsB);
flag = CNodeSetInitStepB(cnode_mem, which, hinB);
flag = CNodeSetMinStepB(cnode_mem, which, hminB);
flag = CNodeSetMaxStepB(cnode_mem, which, hmaxB);
flag = CNodeSetStabLimDetB(cnode_mem, which, stldetB);
```

Their return value `flag` (of type `int`) can have any of the return values of their counterparts, but it can also be `CV_NO_ADJ` if `CNodeAdjInit` has not been called, or `CV_ILL_INPUT` if `which` was an invalid identifier.

### 6.2.8.2 Direct linear solver interface optional input functions

If using a direct linear solver interface for the Jacobian of the backward problem, the linear solver will need to be attached to the memory structure through a call to `CVDlsSetLinearSolverB`. The Jacobian evaluation function can be attached through a call to either `CVDlsSetJacFnB` or `IDACVDlsSetJacFnBS`, with the second used when the backward problem depends on the forward sensitivities.

#### `CVDlsSetJacFnB`

Call `flag = CVDlsSetJacFnB(ida_mem, which, jacB);`

Description The function `CVDlsSetJacFnB` specifies the Jacobian approximation function to be used for the backward problem.

Arguments `cnode_mem` (`void *`) pointer to the CVODES memory returned by `CNodeCreate`.  
`which` (`int`) represents the identifier of the backward problem.  
`jacB` (`CVDlsJacFnB`) user-defined Jacobian approximation function.

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

`CVDLS_SUCCESS` `CVDlsSetJacFnB` succeeded.

`CVDLS_MEM_NULL` `cnode_mem` was `NULL`.

`CVDLS_NO_ADJ` The function `CNodeAdjInit` has not been previously called.

`CVDLS_LMEM_NULL` The linear solver has not been initialized with a call to `CVDlsSetLinearSolverB`.

`CVDLS_ILL_INPUT` The parameter `which` represented an invalid identifier.

Notes The function type `CVDlsJacFnB` is described in §6.3.5.

#### `CVDlsSetJacFnBS`

Call `flag = CVDlsSetJacFnBS(cnode_mem, which, jacBS);`

Description The function `CVDlsSetJacFnBS` specifies the Jacobian approximation function to be used for the backward problem, in the case where the backward problem depends on the forward sensitivities.

Arguments `cnode_mem` (`void *`) pointer to the CVODES memory returned by `CNodeCreate`.  
`which` (`int`) represents the identifier of the backward problem.

|              |   |
|--------------|---|
|              | <code>jacBS</code> (CVDlsJacFnBS) 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> CVDlsSetJacFnBS succeeded.   |
|              | <code>CVDLS_MEM_NULL</code> <code>cvode_mem</code> was NULL.  |
|              | <code>CVDLS_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.                            |
|              | <code>CVDLS_LMEM_NULL</code> The linear solver has not been initialized with a call to <code>CVDlsSetLinearSolverB</code> . |
|              | <code>CVDLS_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier.                            |
| Notes        | The function type <code>CVDlsJacFnBS</code> is described in §6.3.5.   |

### 6.2.8.3 SPILS linear solvers

Optional inputs for the CVSPILS linear solver module can be set for the backward problem through the following functions:

|                                  |   |
|----------------------------------|---|
| <b>CVSpilsSetPreconditionerB</b> |   |
| Call                             | <code>flag = CVSpilsSetPreconditionerB(cvode_mem, which, psetupB, psolveB);</code>  |
| Description                      | The function <code>CVSpilsSetPrecSolveFnB</code> specifies the preconditioner setup and solve functions for the backward integration.   |
| Arguments                        | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>which</code> ( <code>int</code> ) the identifier of the backward problem.<br><code>psetupB</code> ( <code>CVSpilsPrecSetupFnB</code> ) user-defined preconditioner setup function.<br><code>psolveB</code> ( <code>CVSpilsPrecSolveFnB</code> ) 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 value has been successfully set.  |
|                                  | <code>CVSPILS_MEM_NULL</code> <code>cvode_mem</code> was NULL.  |
|                                  | <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.  |
|                                  | <code>CVSPILS_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.  |
|                                  | <code>CVSPILS_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier.  |
| Notes                            | The function types <code>CVSpilsPrecSolveFnB</code> and <code>CVSpilsPrecSetupFnB</code> are described in §6.3.8 and §6.3.9, resp. The <code>psetupB</code> argument may be NULL if no setup operation is involved in the preconditioner.   |

|                                   |   |
|-----------------------------------|---|
| <b>CVSpilsSetPreconditionerBS</b> |   |
| Call                              | <code>flag = CVSpilsSetPreconditionerBS(cvode_mem, which, psetupBS, psolveBS);</code>   |
| Description                       | The function <code>CVSpilsSetPrecSolveFnBS</code> specifies the preconditioner setup and solve functions for the backward integration, in the case where the backward problem depends on the forward sensitivities.   |
| Arguments                         | <code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODES memory block.<br><code>which</code> ( <code>int</code> ) the identifier of the backward problem.<br><code>psetupBS</code> ( <code>CVSpilsPrecSetupFnBS</code> ) user-defined preconditioner setup function.<br><code>psolveBS</code> ( <code>CVSpilsPrecSolveFnBS</code> ) 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 value has been successfully set.  |
|                                   | <code>CVSPILS_MEM_NULL</code> <code>cvode_mem</code> was NULL.  |
|                                   | <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.  |
|                                   | <code>CVSPILS_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.  |

CVSPILS\_ILL\_INPUT The parameter `which` represented an invalid identifier.

Notes The function types `CVSpilsPrecSolveFnBS` and `CVSpilsPrecSetupFnBS` are described in §6.3.8 and §6.3.9, resp. The `psetupBS` argument may be `NULL` if no setup operation is involved in the preconditioner.

#### CVSpilsSetJacTimesB

Call `flag = CVSpilsSetJacTimesB(cvode_mem, which, jsetupB, jtvB);`

Description The function `CVSpilsSetJacTimesB` specifies the Jacobian-vector setup and product functions to be used.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`which` (`int`) the identifier of the backward problem.  
`jtsetupB` (`CVSpilsJacTimesSetupFnB`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.  
`jtvB` (`CVSpilsJacTimesVecFnB`) user-defined Jacobian-vector product function.

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

`CVSPILS_SUCCESS` The optional value has been successfully set.  
`CVSPILS_MEM_NULL` `cvode_mem` was `NULL`.  
`CVSPILS_LMEM_NULL` The CVSPILS linear solver has not been initialized.  
`CVSPILS_NO_ADJ` The function `CVodeAdjInit` has not been previously called.  
`CVSPILS_ILL_INPUT` The parameter `which` represented an invalid identifier.

Notes The function types `CVSpilsJacTimesVecFnB` and `CVSpilsJacTimesSetupFnB` are described in §6.3.6.

#### CVSpilsSetJacTimesBS

Call `flag = CVSpilsSetJacTimesBS(cvode_mem, which, jtvBS);`

Description The function `CVSpilsSetJacTimesBS` specifies the Jacobian-vector setup and product functions to be used, in the case where the backward problem depends on the forward sensitivities.

Arguments `cvode_mem` (`void *`) pointer to the CVODES memory block.  
`which` (`int`) the identifier of the backward problem.  
`jtsetupBS` (`CVSpilsJacTimesSetupFnBS`) user-defined function to set up the Jacobian-vector product. Pass `NULL` if no setup is necessary.  
`jtvBS` (`CVSpilsJacTimesVecFnBS`) user-defined Jacobian-vector product function.

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

`CVSPILS_SUCCESS` The optional value has been successfully set.  
`CVSPILS_MEM_NULL` `cvode_mem` was `NULL`.  
`CVSPILS_LMEM_NULL` The CVSPILS linear solver has not been initialized.  
`CVSPILS_NO_ADJ` The function `CVodeAdjInit` has not been previously called.  
`CVSPILS_ILL_INPUT` The parameter `which` represented an invalid identifier.

Notes The function types `CVSpilsJacTimesVecFnBS` and `CVSpilsJacTimesSetupFnBS` are described in §6.3.6.

**CVSpilsSetEpsLinB**

|              |   |
|--------------|---|
| Call         | <code>flag = CVSpilsSetEpsLinB(cvode_mem, which, eplifacB);</code>  |
| Description  | The function <code>CVSpilsSetEpsLinB</code> specifies the factor by which the Krylov linear solver's convergence test constant is reduced from the Newton iteration test constant. This routine can be used in both the cases where the backward problem does and does not depend on the forward sensitivities.   |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block.<br><code>which</code> (int) the identifier of the backward problem.<br><code>eplifacB</code> (realtype) value of the convergence test constant reduction factor ( $\geq 0.0$ ).   |
| Return value | The return value <code>flag</code> (of type <code>int</code> ) is one of: <ul style="list-style-type: none"> <li><code>CVSPILS_SUCCESS</code> The optional value has been successfully set.</li> <li><code>CVSPILS_MEM_NULL</code> <code>cvode_mem</code> was NULL.</li> <li><code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.</li> <li><code>CVSPILS_NO_ADJ</code> The function <code>CVodeAdjInit</code> has not been previously called.</li> <li><code>CVSPILS_ILL_INPUT</code> The parameter <code>which</code> represented an invalid identifier, or <code>eplifacB</code> was negative.</li> </ul> |
| Notes        | The default value is 0.05. Passing a value <code>eplifacB = 0.0</code> also indicates using the default value.  |

### 6.2.9 Optional output functions for the backward problem

The user of the adjoint module in CVODES has access to any of the optional output functions described in §4.5.8, both for the main solver and for the linear solver modules. The first argument of these `CVodeGet*` and `CVode*Get*` functions is the pointer to the CVODES memory block for the backward problem. In order to call any of these functions, the user must first call the following function to obtain this pointer.

**CVodeGetAdjCVodeBmem**

|              |  |
|--------------|--|
| Call         | <code>cvode_memB = CVodeGetAdjCVodeBmem(cvode_mem, which);</code>  |
| Description  | The function <code>CVodeGetAdjCVodeBmem</code> returns a pointer to the CVODES memory block for the backward problem.  |
| Arguments    | <code>cvode_mem</code> (void *) pointer to the CVODES memory block created by <code>CVodeCreate</code> .<br><code>which</code> (int) the identifier of the backward problem.   |
| Return value | The return value, <code>cvode_memB</code> (of type <code>void *</code> ), is a pointer to the CVODES memory for the backward problem.  |
| Notes        | <p>The user should not modify <code>cvode_memB</code> in any way.</p> <p>Optional output calls should pass <code>cvode_memB</code> as the first argument; for example, to get the number of integration steps: <code>flag = CVodeGetNumSteps(cvodes_memB, &amp;nsteps)</code>.</p> |



To get values of the *forward* solution during a backward integration, use the following function. The input value of `t` would typically be equal to that at which the backward solution has just been obtained with `CVodeGetB`. In any case, it must be within the last checkpoint interval used by `CVodeB`.

**CVodeGetAdjY**

|             |   |
|-------------|---|
| Call        | <code>flag = CVodeGetAdjY(cvode_mem, t, y);</code>  |
| Description | The function <code>CVodeGetAdjY</code> returns the interpolated value of the forward solution <code>y</code> during a backward integration. |
| Arguments   | <code>cvode_mem</code> (void *) pointer to the CVODES memory block created by <code>CVodeCreate</code> .                                    |

|                     |  |
|---------------------|--|
| <b>t</b>            | ( <b>realtype</b> ) value of the independent variable at which $y$ is desired (input). |
| <b>y</b>            | ( <b>N_Vector</b> ) forward solution $y(t)$ .  |
| <b>Return value</b> | The return value <b>flag</b> (of type <b>int</b> ) is one of:                          |
| <b>CV_SUCCESS</b>   | <b>CVodeGetAdjY</b> was successful.  |
| <b>CV_MEM_NULL</b>  | <b>cvode_mem</b> was NULL.   |
| <b>CV_GETY_BADT</b> | The value of <b>t</b> was outside the current checkpoint interval.                     |
| <b>Notes</b>        | The user must allocate space for <b>y</b> .  |



### 6.2.10 Backward integration of quadrature equations

Not only the backward problem but also the backward quadrature equations may or may not depend on the forward sensitivities. Accordingly, either **CVodeQuadInitB** or **CVodeQuadInitBS** should be used to allocate internal memory and to initialize backward quadratures. For any other operation (extraction, optional input/output, reinitialization, deallocation), the same function is callable regardless of whether or not the quadratures are sensitivity-dependent.

#### 6.2.10.1 Backward quadrature initialization functions

The function **CVodeQuadInitB** initializes and allocates memory for the backward integration of quadrature equations that do not depend on forward sensitivities. It has the following form:

##### **CVodeQuadInitB**

|                     |   |
|---------------------|---|
| <b>Call</b>         | <b>flag = CVodeQuadInitB(cvode_mem, which, rhsQB, yQB0);</b>  |
| <b>Description</b>  | The function <b>CVodeQuadInitB</b> provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.  |
| <b>Arguments</b>    | <p><b>cvode_mem</b> (<b>void *</b>) pointer to the CVODES memory block.</p> <p><b>which</b> (<b>int</b>) the identifier of the backward problem.</p> <p><b>rhsQB</b> (<b>CVQuadRhsFnB</b>) is the C function which computes <math>fQB</math>, the right-hand side of the backward quadrature equations. This function has the form <b>rhsQB(t, y, yB, qBdot, user_dataB)</b> (see §6.3.3).</p> <p><b>yQB0</b> (<b>N_Vector</b>) is the value of the quadrature variables at <b>tB0</b>.</p> |
| <b>Return value</b> | The return value <b>flag</b> (of type <b>int</b> ) will be one of the following:  |
| <b>CV_SUCCESS</b>   | The call to <b>CVodeQuadInitB</b> was successful.   |
| <b>CV_MEM_NULL</b>  | <b>cvode_mem</b> was NULL.  |
| <b>CV_NO_ADJ</b>    | The function <b>CVodeAdjInit</b> has not been previously called.  |
| <b>CV_MEM_FAIL</b>  | A memory allocation request has failed.   |
| <b>CV_ILL_INPUT</b> | The parameter <b>which</b> is an invalid identifier.  |

The function **CVodeQuadInitBS** initializes and allocates memory for the backward integration of quadrature equations that depends on the forward sensitivities.

##### **CVodeQuadInitBS**

|                    |  |
|--------------------|--|
| <b>Call</b>        | <b>flag = CVodeQuadInitBS(cvode_mem, which, rhsQBS, yQBS0);</b>  |
| <b>Description</b> | The function <b>CVodeQuadInitBS</b> provides required problem specifications, allocates internal memory, and initializes backward quadrature integration.  |
| <b>Arguments</b>   | <p><b>cvode_mem</b> (<b>void *</b>) pointer to the CVODES memory block.</p> <p><b>which</b> (<b>int</b>) the identifier of the backward problem.</p> <p><b>rhsQBS</b> (<b>CVQuadRhsFnBS</b>) is the C function which computes <math>fQBS</math>, the right-hand side of the backward quadrature equations. This function has the form <b>rhsQBS(t, y, yS, yB, qBdot, user_dataB)</b> (see §6.3.4).</p> |

**yQBS0** (**N\_Vector**) is the value of the sensitivity-dependent quadrature variables at **tB0**.

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

**CV\_SUCCESS** The call to **CVodeQuadInitBS** was successful.  
**CV\_MEM\_NULL** **cvode\_mem** was **NULL**.  
**CV\_NO\_ADJ** The function **CVodeAdjInit** has not been previously called.  
**CV\_MEM\_FAIL** A memory allocation request has failed.  
**CV\_ILL\_INPUT** The parameter **which** is an invalid identifier.

The integration of quadrature equations during the backward phase can be re-initialized by calling the following function. Before calling **CVodeQuadReInitB** for a new backward problem, call any desired solution extraction functions **CVodeGet\*\*** associated with the previous backward problem.

#### **CVodeQuadReInitB**

**Call** **flag = CVodeQuadReInitB(cvode\_mem, which, yQB0);**

**Description** The function **CVodeQuadReInitB** re-initializes the backward quadrature integration.

**Arguments** **cvode\_mem** (**void \***) pointer to the CVODES memory block.  
**which** (**int**) the identifier of the backward problem.  
**yQB0** (**N\_Vector**) is the value of the quadrature variables at **tB0**.

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

**CV\_SUCCESS** The call to **CVodeQuadReInitB** was successful.  
**CV\_MEM\_NULL** **cvode\_mem** was **NULL**.  
**CV\_NO\_ADJ** The function **CVodeAdjInit** has not been previously called.  
**CV\_MEM\_FAIL** A memory allocation request has failed.  
**CV\_NO\_QUAD** Quadrature integration was not activated through a previous call to **CVodeQuadInitB**.  
**CV\_ILL\_INPUT** The parameter **which** is an invalid identifier.

**Notes** The function **CVodeQuadReInitB** can be called after a call to either **CVodeQuadInitB** or **CVodeQuadInitBS**.

#### **6.2.10.2 Backward quadrature extraction function**

To extract the values of the quadrature variables at the last return time of **CVodeB**, CVODES provides a wrapper for the function **CVodeGetQuad** (see §4.7.3). The call to this function has the form

#### **CVodeGetQuadB**

**Call** **flag = CVodeGetQuadB(cvode\_mem, which, &tret, yQB);**

**Description** The function **CVodeGetQuadB** returns the quadrature solution vector after a successful return from **CVodeB**.

**Arguments** **cvode\_mem** (**void \***) pointer to the CVODES memory.  
**tret** (**realtype**) the time reached by the solver (output).  
**yQB** (**N\_Vector**) the computed quadrature vector.

**Return value** The return value **flag** of **CVodeGetQuadB** is one of:

**CV\_SUCCESS** **CVodeGetQuadB** was successful.  
**CV\_MEM\_NULL** **cvode\_mem** is **NULL**.  
**CV\_NO\_ADJ** The function **CVodeAdjInit** has not been previously called.  
**CV\_NO\_QUAD** Quadrature integration was not initialized.  
**CV\_BAD\_DKY** **yQB** was **NULL**.  
**CV\_ILL\_INPUT** The parameter **which** is an invalid identifier.

### 6.2.10.3 Optional input/output functions for backward quadrature integration

Optional values controlling the backward integration of quadrature equations can be changed from their default values through calls to one of the following functions which are wrappers for the corresponding optional input functions defined in §4.7.4. The user must specify the identifier `which` of the backward problem for which the optional values are specified.

```
flag = CNodeSetQuadErrConB(cvode_mem, which, errconQ);
flag = CNodeQuadSStolerancesB(cvode_mem, which, reltolQ, abstolQ);
flag = CNodeQuadSVtolerancesB(cvode_mem, which, reltolQ, abstolQ);
```

Their return value `flag` (of type `int`) can have any of the return values of its counterparts, but it can also be `CV_NO_ADJ` if the function `CNodeAdjInit` has not been previously called or `CV_ILL_INPUT` if the parameter `which` was an invalid identifier.

Access to optional outputs related to backward quadrature integration can be obtained by calling the corresponding `CNodeGetQuad*` functions (see §4.7.5). A pointer `cvode_memB` to the CVODES memory block for the backward problem, required as the first argument of these functions, can be obtained through a call to the functions `CNodeGetAdjCNodeBmem` (see §6.2.9).

## 6.3 User-supplied functions for adjoint sensitivity analysis

In addition to the required ODE right-hand side function and any optional functions for the forward problem, when using the adjoint sensitivity module in CVODES, the user must supply one function defining the backward problem ODE and, optionally, functions to supply Jacobian-related information and one or two functions that define the preconditioner (if one of the CVSPILS solvers is selected) for the backward problem. Type definitions for all these user-supplied functions are given below.

### 6.3.1 ODE right-hand side for the backward problem

If the backward problem does not depend on the forward sensitivities, the user must provide a `rhsB` function of type `CVRhsFnB` defined as follows:

|                 |  |
|-----------------|--|
| <b>CVRhsFnB</b> |  |
| Definition      | <pre>typedef int (*CVRhsFnB)(realtype t, N_Vector y,                         N_Vector yB, N_Vector yBdot, void *user_dataB);</pre>   |
| Purpose         | This function evaluates the right-hand side $f_B(t, y, y_B)$ of the backward problem ODE system. This could be either (2.19) or (2.22).  |
| Arguments       | <p><code>t</code> is the current value of the independent variable.</p> <p><code>y</code> is the current value of the forward solution vector.</p> <p><code>yB</code> is the current value of the backward dependent variable vector.</p> <p><code>yBdot</code> is the output vector containing the right-hand side <math>f_B</math> of the backward ODE problem.</p> <p><code>user_dataB</code> is a pointer to user data, same as passed to <code>CNodeSetUserDataB</code>.</p>  |
| Return value    | A <code>CVRhsFnB</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CNodeB</code> returns <code>CV_RHSFUNC_FAIL</code> ).  |
| Notes           | <p>Allocation of memory for <code>yBdot</code> is handled within CVODES.</p> <p>The <code>y</code>, <code>yB</code>, and <code>yBdot</code> arguments are all of type <code>N_Vector</code>, but <code>yB</code> and <code>yBdot</code> typically have different internal representations from <code>y</code>. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each <code>NVECTOR</code> implementation). For the sake of computational efficiency, the vector</p> |



functions in the two NVECTOR implementations provided with CVODES do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

The `user_dataB` pointer is passed to the user's `rhsB` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `rhsB` function, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the right-hand side function which will halt the integration and `CvodeB` will return `CV_RHSFUNC_FAIL`.

### 6.3.2 ODE right-hand side for the backward problem depending on the forward sensitivities

If the backward problem does depend on the forward sensitivities, the user must provide a `rhsBS` function of type `CVRhsFnBS` defined as follows:

**CVRhsFnBS**

|              |  |  |
|--------------|--|--|
| Definition   | <pre>typedef int (*CVRhsFnBS)(realtype t, N_Vector y, N_Vector *yS,                         N_Vector yB, N_Vector yBdot, void *user_dataB);</pre>  |  |
| Purpose      | This function evaluates the right-hand side $f_B(t, y, y_B, s)$ of the backward problem ODE system. This could be either (2.19) or (2.22).   |  |
| Arguments    | <code>t</code>   | is the current value of the independent variable.  |
|              | <code>y</code>   | is the current value of the forward solution vector.   |
|              | <code>yS</code>  | a pointer to an array of <code>Ns</code> vectors containing the sensitivities of the forward solution. |
|              | <code>yB</code>  | is the current value of the backward dependent variable vector.  |
|              | <code>yBdot</code>   | is the output vector containing the right-hand side $f_B$ of the backward ODE problem.                 |
|              | <code>user_dataB</code> is a pointer to user data, same as passed to <code>CvodeSetUserDataB</code> .  |  |
| Return value | A <code>CVRhsFnBS</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CvodeB</code> returns <code>CV_RHSFUNC_FAIL</code> ). |  |
| Notes        | Allocation of memory for <code>qBdot</code> is handled within CVODES.  |  |

The `y`, `yB`, and `yBdot` arguments are all of type `N_Vector`, but `yB` and `yBdot` typically have different internal representations from `y`. Likewise for each `yS[i]`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each NVECTOR implementation). For the sake of computational efficiency, the vector functions in the two NVECTOR implementations provided with CVODES do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

The `user_dataB` pointer is passed to the user's `rhsBS` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `rhsBS` function, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the right-hand side function which will halt the integration and `CvodeB` will return `CV_RHSFUNC_FAIL`.

### 6.3.3 Quadrature right-hand side for the backward problem

The user must provide an `fQB` function of type `CVQuadRhsFnB` defined by



**CVQuadRhsFnB**

|              |  |  |  |
|--------------|--|--|--|
| Definition   | <pre>typedef int (*CVQuadRhsFnB)(realtype t, N_Vector y, N_Vector yB,                              N_Vector qBdot, void *user_dataB);</pre>  |  |  |
| Purpose      | This function computes the quadrature equation right-hand side for the backward problem.   |  |  |
| Arguments    | t  | is the current value of the independent variable.  |  |
|              | y  | is the current value of the forward solution vector.   |  |
|              | yB   | is the current value of the backward dependent variable vector.                                      |  |
|              | qBdot  | is the output vector containing the right-hand side <b>fQB</b> of the backward quadrature equations. |  |
|              | <b>user_dataB</b> is a pointer to user data, same as passed to <b>CVodeSetUserDataB</b> .  |  |  |
| Return value | A <b>CVQuadRhsFnB</b> should return 0 if successful, a positive value if a recoverable error occurred (in which case <b>CVODES</b> will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <b>CVodeB</b> returns <b>CV_QRHSFUNC_FAIL</b> ).  |  |  |
| Notes        | <p>Allocation of memory for <b>rhsvalBQ</b> is handled within <b>CVODES</b>.</p> <p>The <b>y</b>, <b>yB</b>, and <b>qBdot</b> arguments are all of type <b>N_Vector</b>, but they typically do not all have the same representation. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each <b>NVECTOR</b> implementation). For the sake of computational efficiency, the vector functions in the two <b>NVECTOR</b> implementations provided with <b>CVODES</b> do not perform any consistency checks with respect to their <b>N_Vector</b> arguments (see §7.1 and §7.2).</p> <p>The <b>user_dataB</b> pointer is passed to the user's <b>fQB</b> function every time it is called and can be the same as the <b>user_data</b> pointer used for the forward problem.</p> <p>Before calling the user's <b>fQB</b> function, <b>CVODES</b> needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, <b>CVODES</b> triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and <b>CVodeB</b> will return <b>CV_QRHSFUNC_FAIL</b>.</p> |  |  |



### 6.3.4 Sensitivity-dependent quadrature right-hand side for the backward problem

The user must provide an **fQBS** function of type **CVQuadRhsFnBS** defined by

**CVQuadRhsFnBS**

|            |   |   |  |
|------------|---|---|--|
| Definition | <pre>typedef int (*CVQuadRhsFnBS)(realtype t, N_Vector y, N_Vector *yS,                              N_Vector yB, N_Vector qBdot,                              void *user_dataB);</pre> |   |  |
| Purpose    | This function computes the quadrature equation right-hand side for the backward problem.  |   |  |
| Arguments  | t   | is the current value of the independent variable.   |  |
|            | y   | is the current value of the forward solution vector.  |  |
|            | yS  | a pointer to an array of <b>Ns</b> vectors containing the sensitivities of the forward solution.      |  |
|            | yB  | is the current value of the backward dependent variable vector.                                       |  |
|            | qBdot   | is the output vector containing the right-hand side <b>fQBS</b> of the backward quadrature equations. |  |
|            | <b>user_dataB</b> is a pointer to user data, same as passed to <b>CVodeSetUserDataB</b> .   |   |  |

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

**Notes** Allocation of memory for `qBdot` is handled within CVODES.

The `y`, `yS`, and `qBdot` arguments are all of type `N_Vector`, but they typically do not all have the same internal representation. Likewise for each `yS[i]`. It is the user's responsibility to access the vector data consistently (including the use of the correct accessor macros from each `NVECTOR` implementation). For the sake of computational efficiency, the vector functions in the two `NVECTOR` implementations provided with CVODES do not perform any consistency checks with respect to their `N_Vector` arguments (see §7.1 and §7.2).

The `user_dataB` pointer is passed to the user's `fQBS` function every time it is called and can be the same as the `user_data` pointer used for the forward problem.

Before calling the user's `fQBS` function, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the quadrature right-hand side function which will halt the integration and `CVodeB` will return `CV_QRHSFUNC_FAIL`.



### 6.3.5 Jacobian information for the backward problem (direct method Jacobian)

If the direct linear solver interface is used for the backward problem (i.e. `CVDlsSetLinearSolverB` is called in the step described in §6.1), the user may provide a function of type `CVDlsJacFnB` or `CVDlsJacFnBS` (see §6.2.8), defined as follows:

**CVDlsJacFnB**

**Definition**

```
typedef int (*CVDlsJacFnB)(realtype t, N_Vector y,
                           N_Vector yB, N_Vector fyB,
                           SUNMatrix JacB, void *user_dataB,
                           N_Vector tmp1B, N_Vector tmp2B,
                           N_Vector tmp3B);
```

**Purpose** This function computes the Jacobian of the backward problem (or an approximation to it).

**Arguments**

- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function  $f_B$ .
- `JacB` is the output approximate Jacobian matrix.
- `user_dataB` is a pointer to user data – the same as passed to `CVodeSetUserDataB`.
- `tmp1B`
- `tmp2B`
- `tmp3B` are pointers to memory allocated for variables of type `N_Vector` which can be used by the `CVDlsJacFnB` function as temporary storage or work space.

**Return value** A `CVDlsJacFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES 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, `CVodeB` returns `CV_LSETUP_FAIL` and `CVDLS` sets `last_flag` to `CVDLS_JACFUNC_UNRECVR`).

**Notes** A user-supplied Jacobian function must load the matrix **JacB** with an approximation to the Jacobian matrix at the point  $(t, y, yB)$ , where  $y$  is the solution of the original IVP at time  $tt$ , and  $yB$  is the solution of the backward problem at the same time. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 8 for details). Only nonzero elements need to be loaded into **JacB** as this matrix is set to zero before the call to the Jacobian function.

Before calling the user's **CVDlsJacFnB**, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the Jacobian function which will halt the integration (CVodeB returns **CV\_LSETUP\_FAIL** and CVDLS sets **last\_flag** to **CVDLS\_JACFUNC\_UNRECVR**).



#### CVDlsJacFnBS

**Definition**

```
typedef int (*CVDlsJacFnBS)(realtype t, N_Vector y,
                             N_Vector *yS, N_Vector yB, N_Vector fyB,
                             SUNMatrix JacB, void *user_dataB,
                             N_Vector tmp1B, N_Vector tmp2B,
                             N_Vector tmp3B);
```

**Purpose** This function computes the Jacobian of the backward problem (or an approximation to it), in the case where the backward problem depends on the forward sensitivities.

**Arguments**

- t** is the current value of the independent variable.
- y** is the current value of the forward solution vector.
- yS** a pointer to an array of  $N_s$  vectors containing the sensitivities of the forward solution.
- yB** is the current value of the backward dependent variable vector.
- fyB** is the current value of the backward right-hand side function  $f_B$ .
- JacB** is the output approximate Jacobian matrix.
- user\_dataB** is a pointer to user data – the same as passed to **CVodeSetUserDataB**.
- tmp1B**
- tmp2B**
- tmp3B** are pointers to memory allocated for variables of type **N\_Vector** which can be used by **CVDlsJacFnBS** as temporary storage or work space.

**Return value** A **CVDlsJacFnBS** should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES 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, CVodeB returns **CV\_LSETUP\_FAIL** and CVDLS sets **last\_flag** to **CVDLS\_JACFUNC\_UNRECVR**).

**Notes** A user-supplied Jacobian function must load the matrix **JacB** with an approximation to the Jacobian matrix at the point  $(t, y, yS, yB)$ , where  $y$  is the solution of the original IVP at time  $tt$ ,  $yS$  is the vector of forward sensitivities at time  $tt$ , and  $yB$  is the solution of the backward problem at the same time. Information regarding the structure of the specific SUNMATRIX structure (e.g. number of rows, upper/lower bandwidth, sparsity type) may be obtained through using the implementation-specific SUNMATRIX interface functions (see Chapter 8 for details). Only nonzero elements need to be loaded into **JacB** as this matrix is set to zero before the call to the Jacobian function.

Before calling the user's **CVDlsDenseJacFnBS**, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the Jacobian function which



will halt the integration (CvodeB returns CV\_LSETUP\_FAIL and CVDLS sets last\_flag to CVDLS\_JACFUNC\_UNRECVR).

### 6.3.6 Jacobian information for the backward problem (matrix-vector product)

If the CVSPILS solver interface is selected for the backward problem (i.e., CVSpilsSetLinearSolverB is called in the steps described in §6.1), the user may provide a function of type CVSpilsJacTimesVecFnB or CVSpilsJacTimesVecFnBS 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.

#### CVSpilsJacTimesVecFnB

|              |   |  |
|--------------|---|--|
| Definition   | <pre>typedef int (*CVSpilsJacTimesVecFnB)(N_Vector vB, N_Vector JvB,                                      realtype t, N_Vector y, N_Vector yB,                                      N_Vector fyB, void *user_dataB,                                      N_Vector tmpB);</pre>  |  |
| Purpose      | This function computes the action of the Jacobian JB for the backward problem on a given vector vB.   |  |
| Arguments    | vB  | is the vector by which the Jacobian must be multiplied to the right.   |
|              | JvB   | is the computed output vector JB*vB.   |
|              | t   | is the current value of the independent variable.  |
|              | y   | is the current value of the forward solution vector.   |
|              | yB  | is the current value of the backward dependent variable vector.  |
|              | fyB   | is the current value of the backward right-hand side function $f_B$ .  |
|              | user_dataB  | is a pointer to user data – the same as passed to CvodeSetUserDataB.   |
|              | tmpB  | is a pointer to memory allocated for a variable of type N_Vector which can be used by CVSpilsJacTimesVecFn as temporary storage or work space. |
| Return value | The return value of a function of type CVSpilsJtimesVecFnB should be 0 if successful or nonzero if an error was encountered, in which case the integration is halted.   |  |
| Notes        | A user-supplied Jacobian-vector product function must load the vector JvB with the product of the Jacobian of the backward problem at the point (t,y, yB) and the vector vB. Here, y is the solution of the original IVP at time t and yB is the solution of the backward problem at the same time. The rest of the arguments are equivalent to those passed to a function of type CVSpilsJacTimesVecFn (see §4.6.6). If the backward problem is the adjoint of $\dot{y} = f(t, y)$ , then this function is to compute $-(\partial f / \partial y)^T v_B$ . |  |

#### CVSpilsJacTimesVecFnBS

|            |   |  |
|------------|---|--|
| Definition | <pre>typedef int (*CVSpilsJacTimesVecFnBS)(N_Vector vB, N_Vector JvB,  realtype t, N_Vector y, N_Vector *yS,  N_Vector yB, N_Vector fyB,  void *user_dataB, N_Vector tmpB);</pre> |  |
| Purpose    | This function computes the action of the Jacobian JB for the backward problem on a given vector vB, in the case where the backward problem depends on the forward sensitivities.  |  |
| Arguments  | vB  | is the vector by which the Jacobian must be multiplied to the right. |
|            | JvB   | is the computed output vector JB*vB.                                 |
|            | t   | is the current value of the independent variable.                    |
|            | y   | is the current value of the forward solution vector.                 |
|            | yS  | is a pointer to an array containing the forward sensitivity vectors. |



|              |   |   |
|--------------|---|---|
| Purpose      | This function preprocesses and/or evaluates Jacobian data needed by the Jacobian-times-vector routine for the backward problem, in the case that the backward problem depends on the forward sensitivities.   |   |
| Arguments    | <b>t</b>  | is the current value of the independent variable.   |
|              | <b>y</b>  | is the current value of the dependent variable vector, $y(t)$ .   |
|              | <b>yS</b>   | a pointer to an array of <b>Ns</b> vectors containing the sensitivities of the forward solution.          |
|              | <b>yB</b>   | is the current value of the backward dependent variable vector.   |
|              | <b>fyB</b>  | is the current value of the right-hand-side function for the backward problem.                            |
|              | <b>user_dataB</b>   | is a pointer to user data — the same as the <b>user_dataB</b> parameter passed to <b>CVSetUserDataB</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        | Each call to the Jacobian-vector setup function is preceded by a call to the backward problem residual user function with the same ( <b>t</b> , <b>y</b> , <b>yS</b> , <b>yB</b> ) arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the right-hand-side function.   |   |
|              | If the user's <b>CVSpilsJacTimesVecFnB</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>cvode_mem</b> to <b>user_dataB</b> and then use the <b>CVGet*</b> functions described in §4.5.8.2. The unit roundoff can be accessed as <b>UNIT_ROUNDOFF</b> defined in <b>sundials_types.h</b> . |   |

### 6.3.8 Preconditioning for the backward problem (linear system solution)

If preconditioning is used during integration of the backward problem, then the user must provide a **C** function to solve the linear system  $Pz = r$ , where  $P$  may be either a left or a right preconditioner matrix. Here  $P$  should approximate (at least crudely) the Newton matrix  $M_B = I - \gamma_B J_B$ , where  $J_B = \partial f_B / \partial y_B$ . If preconditioning is done on both sides, the product of the two preconditioner matrices should approximate  $M_B$ . This function must be of one of the following two types:

**CVSpilsPrecSolveFnB**

|            |   |  |
|------------|---|--|
| Definition | <pre>typedef int (*CVSpilsPrecSolveFnB)(realtype t, N_Vector y,                                    N_Vector yB, N_Vector fyB,                                    N_Vector rvecB, N_Vector zvecB,                                    realtype gammaB, realtype deltaB,                                    void *user_dataB);</pre> |  |
| Purpose    | This function solves the preconditioning system $Pz = r$ for the backward problem.  |  |
| Arguments  | <b>t</b>  | is the current value of the independent variable.  |
|            | <b>y</b>  | is the current value of the forward solution vector.   |
|            | <b>yB</b>   | is the current value of the backward dependent variable vector.  |
|            | <b>fyB</b>  | is the current value of the backward right-hand side function $f_B$ .  |
|            | <b>rvecB</b>  | is the right-hand side vector $r$ of the linear system to be solved.   |
|            | <b>zvecB</b>  | is the computed output vector.   |
|            | <b>gammaB</b>   | is the scalar appearing in the Newton matrix, $M_B = I - \gamma_B J_B$ .                                     |
|            | <b>deltaB</b>   | is an input tolerance to be used if an iterative method is employed in the solution.                         |
|            | <b>user_dataB</b>   | is a pointer to user data — the same as the <b>user_dataB</b> parameter passed to <b>CVodeSetUserDataB</b> . |

**Return value** The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

#### CVSpilsPrecSolveFnBS

**Definition** `typedef int (*CVSpilsPrecSolveFnBS)(realtype t, N_Vector y, N_Vector *yS,  
N_Vector yB, N_Vector fyB,  
N_Vector rvecB, N_Vector zvecB,  
realtype gammaB, realtype deltaB,  
void *user_dataB);`

**Purpose** This function solves the preconditioning system  $Pz = r$  for the backward problem, in the case where the backward problem depends on the forward sensitivities.

**Arguments**

- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yS` is a pointer to an array containing the forward sensitivity vectors.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function  $f_B$ .
- `rvecB` is the right-hand side vector  $r$  of the linear system to be solved.
- `zvecB` is the computed output vector.
- `gammaB` is the scalar appearing in the Newton matrix,  $M_B = I - \gamma_B J_B$ .
- `deltaB` is an input tolerance to be used if an iterative method is employed in the solution.
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

**Return value** The return value of a preconditioner solve function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

### 6.3.9 Preconditioning for the backward problem (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 C function of one of the following two types:

#### CVSpilsPrecSetupFnB

**Definition** `typedef int (*CVSpilsPrecSetupFnB)(realtype t, N_Vector y,  
N_Vector yB, N_Vector fyB,  
booleantype jokB, booleantype *jcurPtrB,  
realtype gammaB, void *user_dataB);`

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

**Arguments** The arguments of a `CVSpilsPrecSetupFnB` are as follows:

- `t` is the current value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yB` is the current value of the backward dependent variable vector.
- `fyB` is the current value of the backward right-hand side function  $f_B$ .
- `jokB` is an input flag indicating whether Jacobian-related data needs to be recomputed (`jokB=SUNFALSE`) or information saved from a previous invocation can be safely used (`jokB=SUNTRUE`).



**jcurPtr** is an output flag which must be set to **SUNTRUE** if Jacobian-related data was recomputed or **SUNFALSE** otherwise.

**gammaB** is the scalar appearing in the Newton matrix.

**user\_dataB** is a pointer to user data — the same as the **user\_dataB** parameter passed to **CVodeSetUserDataB**.

**Return value** The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

#### CVSpilsPrecSetupFnBS

**Definition** `typedef int (*CVSpilsPrecSetupFnBS)(realtype t, N_Vector y, N_Vector *yS, N_Vector yB, N_Vector fyB, booleantype jokB, booleantype *jcurPtrB, realtype gammaB, void *user_dataB);`

**Purpose** This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner for the backward problem, in the case where the backward problem depends on the forward sensitivities.

**Arguments** The arguments of a **CVSpilsPrecSetupFnBS** are as follows:

**t** is the current value of the independent variable.

**y** is the current value of the forward solution vector.

**yS** is a pointer to an array containing the forward sensitivity vectors.

**yB** is the current value of the backward dependent variable vector.

**fyB** is the current value of the backward right-hand side function  $f_B$ .

**jokB** is an input flag indicating whether Jacobian-related data needs to be recomputed (**jokB=SUNFALSE**) or information saved from a previous invocation can be safely used (**jokB=SUNTRUE**).

**jcurPtr** is an output flag which must be set to **SUNTRUE** if Jacobian-related data was recomputed or **SUNFALSE** otherwise.

**gammaB** is the scalar appearing in the Newton matrix.

**user\_dataB** is a pointer to user data — the same as the **user\_dataB** parameter passed to **CVodeSetUserDataB**.

**Return value** The return value of a preconditioner setup function for the backward problem should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

## 6.4 Using CVODES preconditioner modules for the backward problem

As on the forward integration phase, the efficiency of Krylov iterative methods for the solution of linear systems can be greatly enhanced through preconditioning. Both preconditioner modules provided with SUNDIALS, the serial banded preconditioner **CVBANDPRE** and the parallel band-block-diagonal preconditioner module **CVBBDPRE**, provide interface functions through which they can be used on the backward integration phase.

### 6.4.1 Using the banded preconditioner CVBANDPRE

The adjoint module in CVODES offers an interface to the banded preconditioner module **CVBANDPRE** described in section §4.8.1. This preconditioner, usable only in a serial setting, provides a band matrix preconditioner based on difference quotients of the backward problem right-hand side function **fB**. It



generates a banded approximation to the Jacobian with  $m_{lB}$  sub-diagonals and  $m_{uB}$  super-diagonals to be used with one of the Krylov linear solvers.

In order to use the CVBANDPRE module in the solution of the backward problem, the user need not define any additional functions. Instead, *after* one of the CVSPILS linear solvers has been specified, by calling the appropriate function (see §6.2.5), the following call to the CVBANDPRE module initialization function must be made.

#### CVBandPrecInitB

|              |   |
|--------------|---|
| Call         | <code>flag = CVBandPrecInitB(cvode_mem, which, nB, muB, mlB);</code>  |
| Description  | The function <code>CVBandPrecInitB</code> initializes and allocates memory for the CVBANDPRE preconditioner for the backward problem. It creates, allocates, and stores (internally in the CVODES solver block) a pointer to the newly created CVBANDPRE memory block.  |
| Arguments    | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>which</code> (int) the identifier of the backward problem.</p> <p><code>nB</code> (sunindextype) backward problem dimension.</p> <p><code>muB</code> (sunindextype) upper half-bandwidth of the backward problem Jacobian approximation.</p> <p><code>mlB</code> (sunindextype) lower half-bandwidth of the backward problem Jacobian approximation.</p>  |
| Return value | <p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CVSPILS_SUCCESS</code> The call to <code>CVodeBandPrecInitB</code> was successful.</p> <p><code>CVSPILS_MEM_FAIL</code> A memory allocation request has failed.</p> <p><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> argument was NULL.</p> <p><code>CVSPILS_LMEM_NULL</code> No linear solver has been attached.</p> <p><code>CVSPILS_ILL_INPUT</code> An invalid parameter has been passed.</p> |

For more details on CVBANDPRE see §4.8.1.

### 6.4.2 Using the band-block-diagonal preconditioner CVBBDPRE

The adjoint module in CVODES offers an interface to the band-block-diagonal preconditioner module CVBBDPRE described in section §4.8.2. This generates a preconditioner that is a block-diagonal matrix with each block being a band matrix and can be used with one of the Krylov linear solvers and with the MPI-parallel vector module NVECTOR\_PARALLEL.

In order to use the CVBBDPRE module in the solution of the backward problem, the user must define one or two additional functions, described at the end of this section.

#### 6.4.2.1 Initialization of CVBBDPRE

The CVBBDPRE module is initialized by calling the following function, *after* one of the CVSPILS linear solvers has been specified by calling the appropriate function (see §6.2.5).

#### CVBBDPrecInitB

|             |   |
|-------------|---|
| Call        | <code>flag = CVBBDPrecInitB(cvode_mem, which, NlocalB, mudqB, mldqB, mukeepB, mlkeepB, dqrelyB, glocB, gcommB);</code>  |
| Description | The function <code>CVBBDPrecInitB</code> initializes and allocates memory for the CVBBDPRE preconditioner for the backward problem. It creates, allocates, and stores (internally in the CVODES solver block) a pointer to the newly created CVBBDPRE memory block. |
| Arguments   | <p><code>cvode_mem</code> (void *) pointer to the CVODES memory block.</p> <p><code>which</code> (int) the identifier of the backward problem.</p> <p><code>NlocalB</code> (sunindextype) local vector dimension for the backward problem.</p>                      |

|                      |  |
|----------------------|--|
| <code>mudqB</code>   | ( <code>sunindextype</code> ) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.   |
| <code>mldqB</code>   | ( <code>sunindextype</code> ) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.   |
| <code>mukeepB</code> | ( <code>sunindextype</code> ) upper half-bandwidth of the retained banded approximate Jacobian block.  |
| <code>mlkeepB</code> | ( <code>sunindextype</code> ) lower half-bandwidth of the retained banded approximate Jacobian block.  |
| <code>dqrelyB</code> | ( <code>realtype</code> ) the relative increment in components of <code>yB</code> used in the difference quotient approximations. The default is <code>dqrelyB</code> = $\sqrt{\text{unit roundoff}}$ , which can be specified by passing <code>dqrely</code> = 0.0. |
| <code>glocB</code>   | ( <code>CVBBDLocalFnB</code> ) the C function which computes the function $g_B(t, y, y_B)$ approximating the right-hand side of the backward problem.  |
| <code>gcommB</code>  | ( <code>CVBBDCommFnB</code> ) the optional C function which performs all interprocess communication required for the computation of $g_B$ .  |

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

|                                |  |
|--------------------------------|--|
| <code>CVSPILS_SUCCESS</code>   | The call to <code>CVodeBBDPrecInitB</code> was successful. |
| <code>CVSPILS_MEM_FAIL</code>  | A memory allocation request has failed.                    |
| <code>CVSPILS_MEM_NULL</code>  | The <code>cvode_mem</code> argument was NULL.              |
| <code>CVSPILS_LMEM_NULL</code> | No linear solver has been attached.                        |
| <code>CVSPILS_ILL_INPUT</code> | An invalid parameter has been passed.                      |

To reinitialize the CVBBDPRE preconditioner module for the backward problem, possibly with changes in `mudqB`, `mldqB`, or `dqrelyB`, call the following function:

#### `CVBBDPrecReInitB`

|             |   |
|-------------|---|
| Call        | <code>flag = CVBBDPrecReInitB(cvode_mem, which, mudqB, mldqB, dqrelyB);</code>  |
| Description | The function <code>CVBBDPrecReInitB</code> reinitializes the CVBBDPRE preconditioner for the backward problem.  |
| Arguments   | <p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODES memory block returned by <code>CVodeCreate</code>.</p> <p><code>which</code> (<code>int</code>) the identifier of the backward problem.</p> <p><code>mudqB</code> (<code>sunindextype</code>) upper half-bandwidth to be used in the difference-quotient Jacobian approximation.</p> <p><code>mldqB</code> (<code>sunindextype</code>) lower half-bandwidth to be used in the difference-quotient Jacobian approximation.</p> <p><code>dqrelyB</code> (<code>realtype</code>) the relative increment in components of <code>yB</code> used in the difference quotient approximations.</p> |

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

|                                |  |
|--------------------------------|--|
| <code>CVSPILS_SUCCESS</code>   | The call to <code>CVodeBBDPrecReInitB</code> was successful.       |
| <code>CVSPILS_MEM_FAIL</code>  | A memory allocation request has failed.                            |
| <code>CVSPILS_MEM_NULL</code>  | The <code>cvode_mem</code> argument was NULL.                      |
| <code>CVSPILS_PMEM_NULL</code> | The <code>CVodeBBDPrecInitB</code> has not been previously called. |
| <code>CVSPILS_LMEM_NULL</code> | No linear solver has been attached.                                |
| <code>CVSPILS_ILL_INPUT</code> | An invalid parameter has been passed.                              |

For more details on CVBBDPRE see §4.8.2.

### 6.4.2.2 User-supplied functions for CVBBDPRE

To use the CVBBDPRE module, the user must supply one or two functions which the module calls to construct the preconditioner: a required function `glocB` (of type `CVBBDLocalFnB`) which approximates the right-hand side of the backward problem and which is computed locally, and an optional function `gcommB` (of type `CVBBDCommFnB`) which performs all interprocess communication necessary to evaluate this approximate right-hand side (see §4.8.2). The prototypes for these two functions are described below.

#### CVBBDLocalFnB

**Definition** `typedef int (*CVBBDLocalFnB)(sunindextype NlocalB, realtype t, N_Vector y, N_Vector yB, N_Vector gB, void *user_dataB);`

**Purpose** This `glocB` function loads the vector `gB`, an approximation to the right-hand side  $f_B$  of the backward problem, as a function of `t`, `y`, and `yB`.

**Arguments**

- `NlocalB` is the local vector length for the backward problem.
- `t` is the value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yB` is the current value of the backward dependent variable vector.
- `gB` is the output vector,  $g_B(t, y, y_B)$ .
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

**Return value** An `CVBBDLocalFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_LSETUP_FAIL`).

**Notes** This routine must assume that all interprocess communication of data needed to calculate `gB` has already been done, and this data is accessible within `user_dataB`.

Before calling the user's `CVBBDLocalFnB`, CVODES needs to evaluate (through interpolation) the values of the states from the forward integration. If an error occurs in the interpolation, CVODES triggers an unrecoverable failure in the preconditioner setup function which will halt the integration (`CVodeB` returns `CV_LSETUP_FAIL`).



#### CVBBDCommFnB

**Definition** `typedef int (*CVBBDCommFnB)(sunindextype NlocalB, realtype t, N_Vector y, N_Vector yB, void *user_dataB);`

**Purpose** This `gcommB` function must perform all interprocess communications necessary for the execution of the `glocB` function above, using the input vectors `y` and `yB`.

**Arguments**

- `NlocalB` is the local vector length.
- `t` is the value of the independent variable.
- `y` is the current value of the forward solution vector.
- `yB` is the current value of the backward dependent variable vector.
- `user_dataB` is a pointer to user data — the same as the `user_dataB` parameter passed to `CVodeSetUserDataB`.

**Return value** An `CVBBDCommFnB` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODES will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVodeB` returns `CV_LSETUP_FAIL`).

## Notes

The `gcommB` function is expected to save communicated data in space defined within the structure `user_dataB`.

Each call to the `gcommB` function is preceded by a call to the function that evaluates the right-hand side of the backward problem with the same `t`, `y`, and `yB`, arguments. If there is no additional communication needed, then pass `gcommB = NULL` to `CVBBDPrecInitB`.

## Chapter 7

# 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   (*nvintest)(N_Vector, N_Vector);
boolean_t   (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
realtype    (*nvminquotient)(N_Vector, N_Vector);
};

```

The generic NVECTOR module defines and implements the vector operations acting on `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 7.2 contains a complete list of all vector operations defined by the generic NVECTOR module.

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:

- 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 7.1. It is recommended that a user-supplied NVECTOR implementation use the `SUNDIALS_NVEC_CUSTOM` identifier.

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

| Vector ID              | Vector type                         | ID Value |
|------------------------|-------------------------------------|----------|
| SUNDIALS_NVEC_SERIAL   | Serial                              | 0        |
| SUNDIALS_NVEC_PARALLEL | Distributed memory parallel (MPI)   | 1        |
| SUNDIALS_NVEC_OPENMP   | OpenMP shared memory parallel       | 2        |
| SUNDIALS_NVEC_PTHREADS | PThreads shared memory parallel     | 3        |
| SUNDIALS_NVEC_PARHYP   | <i>hypre</i> ParHyp parallel vector | 4        |
| SUNDIALS_NVEC_PETSC    | PETSc parallel vector               | 5        |
| SUNDIALS_NVEC_CUSTOM   | User-provided custom vector         | 6        |

Table 7.2: Description of the NVECTOR operations

| Name                   | Usage and Description   |
|------------------------|---|
| N_VGetVectorID         | <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 7.1.  |
| N_VClone               | <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.   |
| N_VCloneEmpty          | <code>v = N_VCloneEmpty(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 allocate storage for data.   |
| N_VDestroy             | <code>N_VDestroy(v);</code><br>Destroys the <code>N_Vector</code> <code>v</code> 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 <code>N_Vector</code> . <code>lrw</code> contains the number of realtype words and <code>liw</code> 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. |
| continued on next page |   |

| <i>continued from last page</i> |  |
|---------------------------------|--|
| Name                            | Usage and Description  |
| N_VGetArrayPointer              | <pre>vdata = N_VGetArrayPointer(v);</pre> <p>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.</p> |
| N_VSetArrayPointer              | <pre>N_VSetArrayPointer(vdata, v);</pre> <p>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.</p>  |
| N_VLinearSum                    | <pre>N_VLinearSum(a, x, b, y, z);</pre> <p>Performs the operation <math>z = ax + by</math>, where <math>a</math> and <math>b</math> are <b>realtype</b> scalars and <math>x</math> and <math>y</math> are of type <b>N_Vector</b>: <math>z_i = ax_i + by_i</math>, <math>i = 0, \dots, n-1</math>.</p>   |
| N_VConst                        | <pre>N_VConst(c, z);</pre> <p>Sets all components of the <b>N_Vector</b> <b>z</b> to <b>realtype</b> <math>c</math>: <math>z_i = c</math>, <math>i = 0, \dots, n-1</math>.</p>   |
| N_VProd                         | <pre>N_VProd(x, y, z);</pre> <p>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>: <math>z_i = x_i y_i</math>, <math>i = 0, \dots, n-1</math>.</p>  |
| N_VDiv                          | <pre>N_VDiv(x, y, z);</pre> <p>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                        | <pre>N_VScale(c, x, z);</pre> <p>Scales the <b>N_Vector</b> <b>x</b> by the <b>realtype</b> scalar <math>c</math> and returns the result in <b>z</b>: <math>z_i = cx_i</math>, <math>i = 0, \dots, n-1</math>.</p>   |
| N_VAbs                          | <pre>N_VAbs(x, z);</pre> <p>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>z_i =  x_i </math>, <math>i = 0, \dots, n-1</math>.</p>   |
| <i>continued on next page</i>   |  |



| <i>continued from last page</i> |   |
|---------------------------------|---|
| Name                            | Usage and Description   |
| N_VInv                          | <p><code>N_VInv(x, z);</code><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><code>N_VAddConst(x, b, z);</code><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><code>d = N_VDotProd(x, y);</code><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><code>m = N_VMaxNorm(x);</code><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><code>m = N_VWrmsNorm(x, w)</code><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><code>m = N_VWrmsNormMask(x, w, id);</code><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 nonzero 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 \text{sign}(id_i))^2) / n}.</math></p> |
| N_VMin                          | <p><code>m = N_VMin(x);</code><br/> Returns the smallest element of the <b>N_Vector</b> <b>x</b>: <math>m = \min_i x_i</math>.</p>  |
| N_VWL2Norm                      | <p><code>m = N_VWL2Norm(x, w);</code><br/> Returns the weighted Euclidean <math>\ell_2</math> 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}</math>.</p>   |
| N_VL1Norm                       | <p><code>m = N_VL1Norm(x);</code><br/> Returns the <math>\ell_1</math> norm of the <b>N_Vector</b> <b>x</b>: <math>m = \sum_{i=0}^{n-1}  x_i </math>.</p>   |
| N_VCompare                      | <p><code>N_VCompare(c, x, z);</code><br/> Compares the components of the <b>N_Vector</b> <b>x</b> to the <b>realtype</b> scalar <b>c</b> and returns an <b>N_Vector</b> <b>z</b> such that: <math>z_i = 1.0</math> if <math> x_i  \geq c</math> and <math>z_i = 0.0</math> otherwise.</p>   |
| <i>continued on next page</i>   |   |

| continued from last page |   |
|--------------------------|---|
| Name                     | Usage and Description   |
| N_VInvTest               | <code>t = N_VInvTest(x, z);</code><br>Sets the components of the <code>N_Vector</code> <code>z</code> to be the inverses of the components of the <code>N_Vector</code> <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.  |

## 7.1 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 Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Serial` (e.g. `NV_Destroy_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.

## 7.2 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.

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

Implementation:

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

These macros give individual access to the parts of the content of a parallel N\_Vector.

The assignment `vllen = NV_LOCLENGTH.P(v)` sets `vllen` to be the length of the local part of `v`. The call `NV_LENGTH.P(v) = llen_v` sets the local length of `v` to be `llen_v`.

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

Implementation:

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

This macro provides access to the MPI communicator used by the NVECTOR\_PARALLEL vectors.

Implementation:

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

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

The assignment  $\mathbf{r} = \text{NV\_Ith\_P}(\mathbf{v}, i)$  sets  $\mathbf{r}$  to be the value of the  $i$ -th component of the local part of  $\mathbf{v}$ . The assignment  $\text{NV\_Ith\_P}(\mathbf{v}, i) = \mathbf{r}$  sets the value of the  $i$ -th component of the local part of  $\mathbf{v}$  to be  $\mathbf{r}$ .

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

Implementation:

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

The `NVECTOR_PARALLEL` module defines parallel implementations of all vector operations listed in Table 7.2. Their names are obtained from those in Table 7.2 by appending the suffix `_Parallel` (e.g. `N_VDestroy_Parallel`). The module `NVECTOR_PARALLEL` provides the following additional user-callable routines:

This function creates and allocates memory for a parallel vector.

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

- `N_VNewEmpty_Parallel`

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

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

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

## 7.3 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;
    booleantype own_data;
    realtype *data;
    int num_threads;
};
```

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

The 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 Table 7.2. Their names are obtained from those in Table 7.2 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 `FNVINITOMP(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for `CVODE`, 2 for `IDA`, 3 for `KINSOL`, 4 for `ARKODE`); `NEQ` is the problem size (declared so as to match C type `long int`); `NUMTHREADS` is the number of threads; and `IER` is an error return flag equal 0 for success and -1 for failure.

## 7.4 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_nvec_pthreads.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 Table 7.2. Their names are obtained from those in Table 7.2 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 `FNINITPTS(code, NEQ, NUMTHREADS, IER)`, to initialize this module. Here `code` is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); `NEQ` is the problem size (declared so as to match C type `long int`); `NUMTHREADS` is the number of threads; and `IER` is an error return flag equal 0 for success and -1 for failure.

## 7.5 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 `hypre_ParVector, an MPI communicator, and a boolean flag own_parvector indicating ownership of the hypre parallel vector object x.`

```
struct _N_VectorContent_ParHyp {
    sunindextype local_length;
    sunindextype global_length;
    booleantype own_parvector;
    MPI_Comm comm;
    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 Table 7.2, 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 [23] and the `ark_diurnal_kry_ph.c` example program for ARKODE [31].

The names of parhyp methods are obtained from those in Table 7.2 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 *hypre* vector.

```
hypre_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 *hypre* vector via `x_vec = N_VGetVector_ParHyp(v)` and then access components using appropriate *hypre* functions.
- `N_VNewEmpty_ParHyp`, `N_VMake_ParHyp`, and `N_VCloneVectorArrayEmpty_ParHyp` set the field *own\_parvector* to `SUNFALSE`. `N_VDestroy_ParHyp` and `N_VDestroyVectorArray_ParHyp` will not attempt to delete an underlying *hypre* vector for any `N_Vector` with *own\_parvector* set to `SUNFALSE`. In such a case, it is the user's responsibility to delete the underlying vector.
- To maximize efficiency, vector operations in the `NVECTOR_PARHYP` implementation that have more than one `N_Vector` argument do not check for consistent internal representations of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.



## 7.6 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;
    booleantype own_data;
    Vec *pvec;
    MPI_Comm comm;
};

```

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

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

The NVECTOR\_PETSC module defines implementations of all vector operations listed in Table 7.2, 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 [22].

The names of vector operations are obtained from those in Table 7.2 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_VCloneEmptyVectorArray_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.



## 7.7 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 Table 7.2, 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 [23].

The names of vector operations are obtained from those in Table 7.2 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_VCloneEmptyVectorArray_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.



## 7.8 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 `sunrajavec::Vector` class will change frequently in future SUNDIALS releases. The code is structured so that it can tolerate significant changes in the `sunrajavec::Vector` class without requiring changes to the user API.

The header file to include when using this module is `nvector_raja.h`. The installed module library to link to 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 Table 7.2, 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. 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 [23].

The names of vector operations are obtained from those in Table 7.2 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 `sunrajavec::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_VCloneEmptyVectorArray_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.



## 7.9 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 max norm.
- **Test\_N\_VWrmsNorm**: Create vector of known values, find and validate weighted root mean square.
- **Test\_N\_VWrmsNormMask**: Case 1: Create vector of known values, find and validate weighted root mean square using all elements.
- **Test\_N\_VWrmsNormMask**: Case 2: Create vector of known values, find and validate weighted root mean square using no elements.
- **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.

## 7.10 NVECTOR functions used by CVODES

In Table 7.3 below, we list the vector functions in the NVECTOR module used within the CVODES package. The table also shows, for each function, which of the code modules uses the function. The CVODES column shows function usage within the main integrator module, while the remaining columns show function usage within each of the CVODES linear solver interfaces, the CVBANDPRE and CVBBDPRE preconditioner modules, and the CVODES adjoint sensitivity module (denoted here by CVODEA). Here CVDLS stands for the direct linear solver interface in CVODES; CVSPILS stands for the scaled, preconditioned, iterative linear solver interface in CVODES.

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

The vector functions listed in Table 7.2 that are *not* used by CVODES are: `N_VWL2Norm`, `N_VL1Norm`, `N_VWrmsNormMask`, `N_VConstrMask`, `N_VCloneEmpty`, and `N_VMinQuotient`. Therefore, a user-supplied NVECTOR module for CVODES could omit these six kernels.

Table 7.3: List of vector functions usage by CVOIDES code modules

|                       | CVOIDES | CVDLS | CVDIAG | CVSPILS | CVBANDPRE | CVBBDPRE | CVODEA |
|-----------------------|---------|-------|--------|---------|-----------|----------|--------|
| N_GetVectorID         |         |       |        |         |           |          |        |
| N_VClone              | ✓       |       | ✓      | ✓       |           |          | ✓      |
| N_VDestroy            | ✓       |       | ✓      | ✓       |           |          | ✓      |
| N_VCloneVectorArray   | ✓       |       |        |         |           |          | ✓      |
| N_VDestroyVectorArray | ✓       |       |        |         |           |          | ✓      |
| 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            |         |       | ✓      |         |           |          |        |

## Chapter 8

# Description of the SUNMatrix module

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

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 8.1: 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 8.2 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 8.1. It is recommended that a user-supplied SUNMATRIX implementation use the `SUNMATRIX_CUSTOM` identifier.

Table 8.2: Description of the `SUNMatrix` operations

| Name                          | Usage and Description  |
|-------------------------------|--|
| SUNMatGetID                   | <code>id = SUNMatGetID(A);</code><br>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 8.1. |
| <i>continued on next page</i> |  |



| Name            | Usage and Description  |
|-----------------|--|
| SUNMatClone     | <p><code>B = SUNMatClone(A);</code><br/> 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   | <p><code>SUNMatDestroy(A);</code><br/> Destroys the <b>SUNMatrix</b> <b>A</b> and frees memory allocated for its internal data.</p>  |
| SUNMatSpace     | <p><code>ier = SUNMatSpace(A, &amp;lrw, &amp;liw);</code><br/> 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.<br/> 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      | <p><code>ier = SUNMatZero(A);</code><br/> 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      | <p><code>ier = SUNMatCopy(A,B);</code><br/> 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  | <p><code>ier = SUNMatScaleAdd(c, A, B);</code><br/> Performs the operation <math>A = cA + B</math>. The return value is an integer flag denoting success/failure of the operation.</p>   |
| SUNMatScaleAddI | <p><code>ier = SUNMatScaleAddI(c, A);</code><br/> Performs the operation <math>A = cA + I</math>. The return value is an integer flag denoting success/failure of the operation.</p>   |
| SUNMatMatvec    | <p><code>ier = SUNMatMatvec(A, x, y);</code><br/> 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 9. More specifically, in Table 8.3 we show the matrix interfaces available as `SUNMATRIX` modules, and the compatible vector implementations.

Table 8.3: SUNDIALS matrix interfaces and vector implementations that can be used for each.

| Matrix Interface | Serial | Parallel (MPI) | OpenMP | pThreads | 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    | ✓      | ✓              | ✓      | ✓        | ✓          | ✓          | ✓    | ✓    | ✓           |

## 8.1 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 8.2. Their names are obtained from those in Table 8.2 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.

## 8.2 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 8.1. A more complete description of the parts of this *content* field is given below:

**M** - number of rows

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

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

**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 ( $ldim \geq s\_mu$ )

**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 ( $= ldim \cdot (s\_mu + ml + 1)$ )

**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.

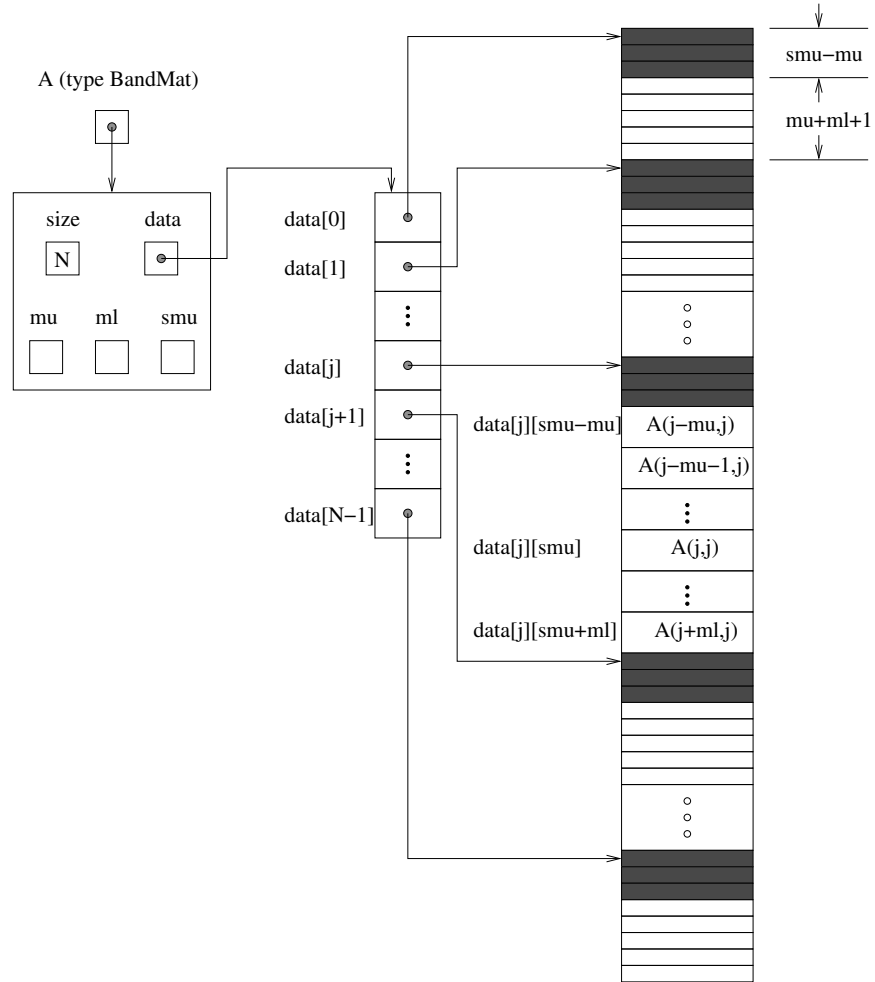


Figure 8.1: Diagram of the storage for the SUNMATRIX\_BAND module. Here  $A$  is an  $N \times N$  band matrix with upper and lower half-bandwidths  $\mu$  and  $m_l$ , respectively. The rows and columns of  $A$  are numbered from 0 to  $N - 1$  and the  $(i, j)$ -th element of  $A$  is denoted  $A(i, j)$ . 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_SUBAND_B(A) )
#define SM_COLUMN_ELEMENT_B(col_j,i,j) (col_j[(i)-(j)])
#define SM_ELEMENT_B(A,i,j)
    ( (SM_CONTENT_B(A)->cols)[j][(i)-(j)+SM_SUBAND_B(A)] )
```

The `SUNMATRIX_BAND` module defines banded implementations of all matrix operations listed in Table 8.2. Their names are obtained from those in Table 8.2 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`, if the matrix will be used by the `SUNLINSOL_BAND` module then `smu` should be at least  $\min(N-1, \mu+ml)$ ; otherwise `smu` should be at least `mu`.

```
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  $m_l$ .

```
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.

## 8.3 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 8.2 (the CSR format is similar). A more complete description of the parts of this *content* field is given below:

**M** - number of rows

**N** - number of columns

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

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

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

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

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

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

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

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

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

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

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

For example, the  $5 \times 4$  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) )
```

- `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`.

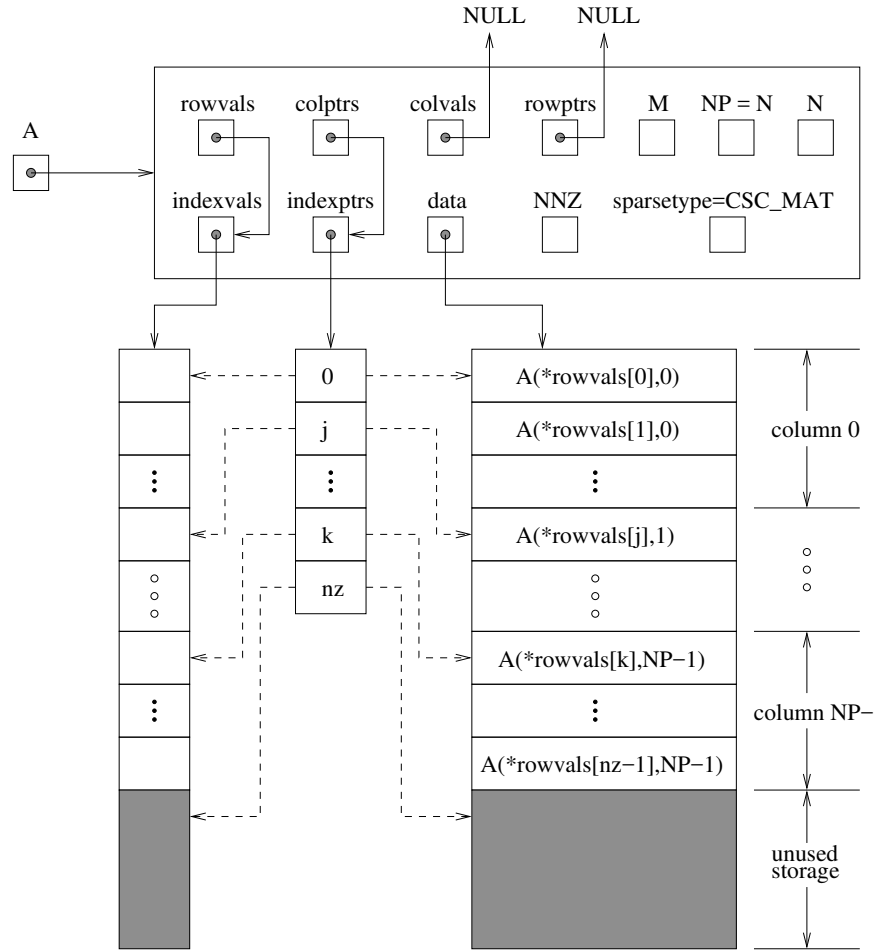


Figure 8.2: Diagram of the storage for a compressed-sparse-column matrix. Here  $A$  is an  $M \times N$  sparse matrix with storage for up to  $NNZ$  nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 0 to  $M - 1$ , corresponding 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.

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 8.2. Their names are obtained from those in Table 8.2 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\_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.



## 8.4 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`.

## 8.5 SUNMatrix functions used by CVODES

In Table 8.4 below, we list the matrix functions in the SUNMATRIX module used within the CVODES package. The table also shows, for each function, which of the code modules uses the function. Neither the main CVODES 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 CVODES user does not need to know anything about the usage of matrix functions by the CVODES code modules in order to use CVODES. The information is presented as an implementation detail for the interested reader.

Table 8.4: List of matrix functions usage by CVODES code modules

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

The matrix functions listed in Table 8.2 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 8.2 that are *not* used by CVODES are: `SUNMatScaleAdd` and `SUNMatMatvec`. Therefore a user-supplied SUNMATRIX module for CVODES could omit these functions.



## Chapter 9

# 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

$$\tilde{A}\tilde{x} = \tilde{b} \tag{9.1}$$

where

$$\begin{aligned} \tilde{A} &= S_1 P_1^{-1} A P_2^{-1} S_2^{-1}, \\ \tilde{b} &= S_1 P_1^{-1} b, \\ \tilde{x} &= S_2 P_2 x, \end{aligned} \tag{9.2}$$

and where

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

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 9.2 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 9.1: 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 9.1. 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 9.2: 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 9.1. |

*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 9.4.</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 9.4.</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 9.4.</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 9.4.</p>   |
| continued on next page |   |

| 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 (9.1)-(9.2). 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 9.4.</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 (9.1)-(9.2). Similarly, s2 is an NVECTOR containing the diagonal of <math>S_2</math> from equations (9.1)-(9.2). 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 9.4.</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. |

## 9.1 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

## 9.2 Compatibility of SUNLinearSolver modules

We note that not all SUNLINSOL types are compatible with all SUNMATRIX and NVECTOR types provided with SUNDIALS. In Table 9.3 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 9.3: 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 9.4.

Table 9.4: 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> )   |

### 9.3 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 9.2:

- `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.

## 9.4 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 9.2:

- `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.

## 9.5 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 9.2:

- `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.

## 9.6 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 9.2:

- `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.

## 9.7 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, 11]. 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 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 9.2:

- `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:

- 1 The Jacobian matrix will be destroyed and a new one will be allocated based on the `nnz` value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.
- 2 Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of `nnz` given in the sparse matrix provided to the original constructor routine (or the previous `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`
- `FSUNMassKLUReInit(NNZ, reinit_type, ier)`
- `FSUNKLUSetOrdering(code, ordering, ier)` – `ordering` should be commensurate with a C `int`
- `FSUNMassKLUSetOrdering(ordering, ier)`

## 9.8 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, 27, 12]. 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 9.2:

- `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)`

## 9.9 The SUNLinearSolver\_SPGMR implementation

The SPGMR (Scaled, Preconditioned, Generalized Minimum Residual [33]) 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 9.2:

- `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)`

## 9.10 The SUNLinearSolver\_SPFGMR implementation

The SPFGMR (Scaled, Preconditioned, Flexible, Generalized Minimum Residual [32]) 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  $z_1, \dots, z_{\maxl+1}$ , stored in `Z[0], \dots, Z[\maxl]`. Each  $z_i$  is a vector of type `NVECTOR`.,

**Hes** - the  $(\maxl + 1) \times \maxl$  Hessenberg matrix. It is stored row-wise so that the  $(i,j)$ th element is given by `Hes[i][j]`.,

**givens** - a length  $2*\maxl$  array which represents the Givens rotation matrices that arise in the 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  $(\maxl+1)$  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 9.2:

- `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)`

## 9.11 The SUNLinearSolver\_SPBCGS implementation

The SPBCGS (Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [36]) 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 9.2:

- `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)`

## 9.12 The SUNLinearSolver\_SPTFQMR implementation

The SPTFQMR (Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [14]) 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 9.2:

- `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)

## 9.13 The SUNLinearSolver\_PCG implementation

The PCG (Preconditioned Conjugate Gradient [15]) 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

$$\tilde{A}\tilde{x} = \tilde{b} \quad (9.3)$$

where

$$\begin{aligned} \tilde{A} &= SP^{-1}AP^{-1}S, \\ \tilde{b} &= SP^{-1}b, \\ \tilde{x} &= S^{-1}Px. \end{aligned} \quad (9.4)$$

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 9.2:

- `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)`

## 9.14 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  $10 * \text{tol}$ , 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.

## 9.15 SUNLinearSolver functions used by CVODES

In Table 9.5 below, we list the linear solver functions in the SUNLINSOL module used within the CVODES package. The table also shows, for each function, which of the code modules uses the function. In general, the main CVODES integrator considers three categories of linear solvers, *direct*, *iterative* and *custom*, with interfaces accessible in the CVODES header files **cvodes\_direct.h** (CVDLS), **cvodes\_spils.h** (CVSPILS) and **cvodes\_customls.h** (CVCLS), respectively. Hence, the the table columns reference the use of SUNLINSOL functions by each of these solver interfaces.

As with the SUNMATRIX module, we emphasize that the CVODES user does not need to know detailed usage of linear solver functions by the CVODES code modules in order to use CVODES. The information is presented as an implementation detail for the interested reader.

Table 9.5: List of linear solver functions usage by CVODES code modules

|                                   | CVDLS | CVSPILS | CVCLS |
|-----------------------------------|-------|---------|-------|
| <b>SUNLinSolGetType</b>           | ✓     | ✓       | †     |
| <b>SUNLinSolSetATimes</b>         |       | ✓       | †     |
| <b>SUNLinSolSetPreconditioner</b> |       | ✓       | †     |
| <b>SUNLinSolSetScalingVectors</b> |       | ✓       | †     |
| <b>SUNLinSolInitialize</b>        | ✓     | ✓       | ✓     |
| <b>SUNLinSolSetup</b>             | ✓     | ✓       | ✓     |
| <b>SUNLinSolSolve</b>             | ✓     | ✓       | ✓     |
| <b>SUNLinSolNumIters</b>          |       | ✓       | †     |
| <b>SUNLinSolResNorm</b>           |       | ✓       | †     |
| <b>SUNLinSolResid</b>             |       | ✓       | †     |
| <b>SUNLinSolLastFlag</b>          |       |         |       |
| <b>SUNLinSolFree</b>              | ✓     | ✓       | ✓     |
| <b>SUNLinSolSpace</b>             | †     | †       | †     |

The linear solver functions listed in Table 9.2 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 CVODES does not call the `SUNLinSolLastFlag` directly, this routine is available for users to query linear solver issues directly.

## 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:

***srcdir*** 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 *srcdir* 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 *srcdir*.
- 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 2.8.1 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 is probably out of date. Many new CMake features have been added recently, and you should download the latest version 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 *installdir* 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/instldir
% 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 *srcdir*:

```
% ccmake ../srcdir
```

The default configuration screen is shown in Figure A.1.

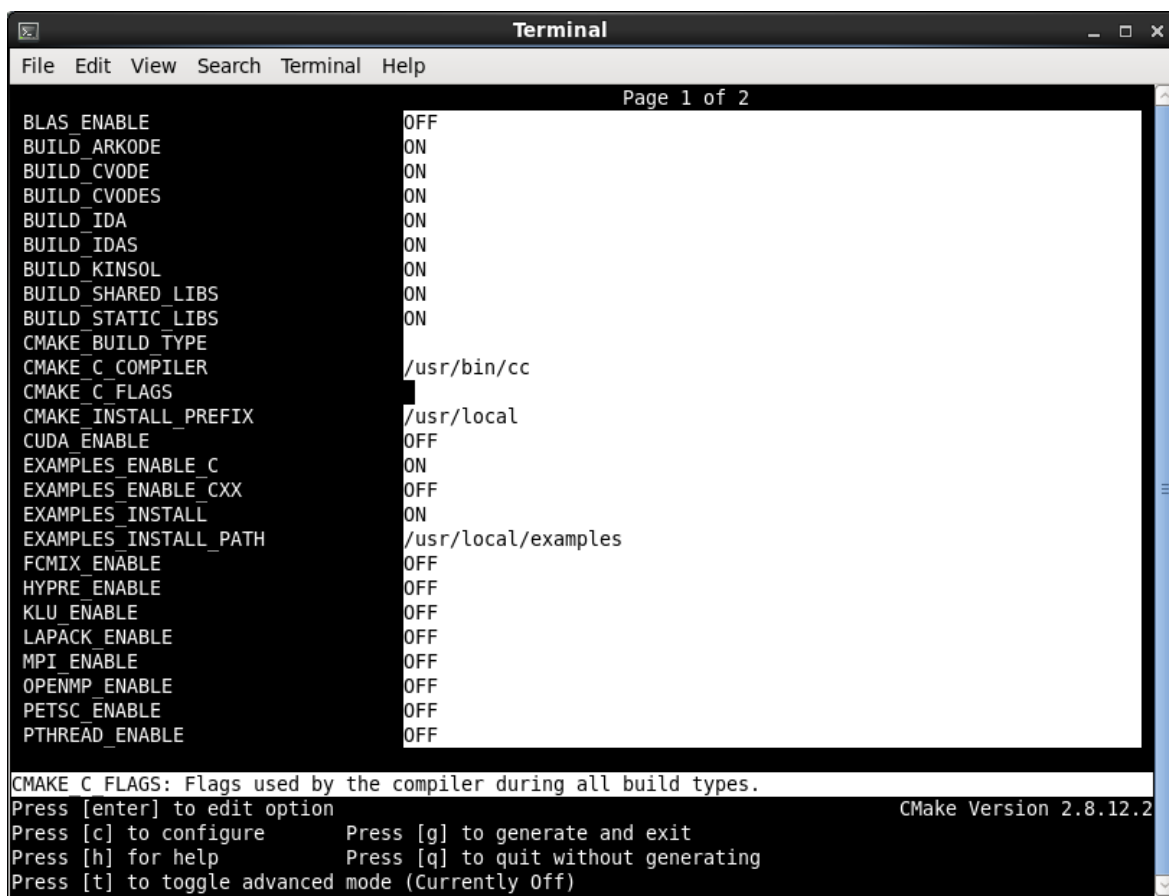


Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

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
```

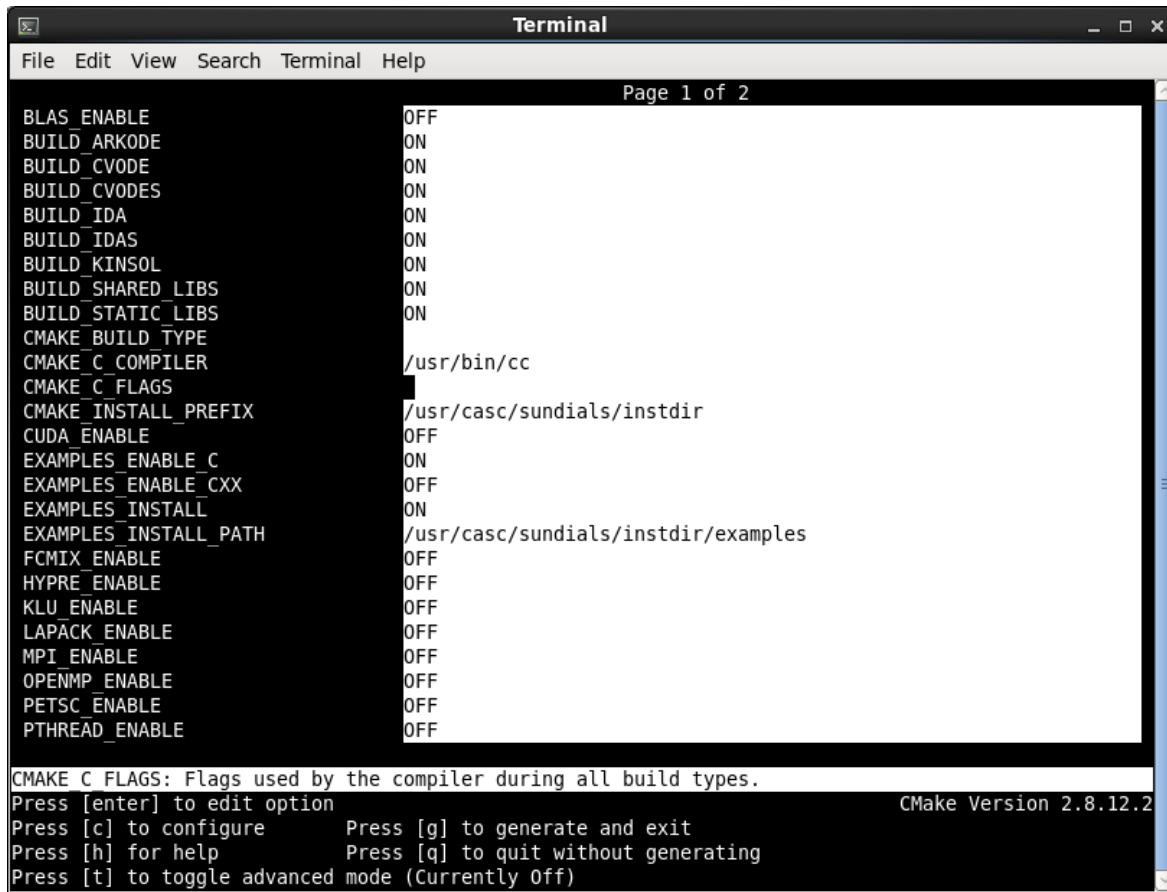


Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

### 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 \
> ../srcdir
% 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_MPICC` - `mpicc` program

Default:

`MPI_MPICXX` - `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_MPIF77` - `mpif77` program

Default:

Note: This option is triggered only if MPI is enabled (`MPI_ENABLE` is `ON`) and Fortran-C support is enabled (`FCMIX_ENABLE` is `ON`).

**MPI\_MPIF90** - 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 Fortran90 examples are enabled (**EXAMPLES\_ENABLE\_F90** is ON).

**MPI\_RUN\_COMMAND** - Specify run command for MPI

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\_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/srcdir  
%  
% 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/srcdir  
%  
% 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 build 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/srcdir
%
% make install
%
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.



### 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/srcdir
%
% make install
%
```

If enabling LAPACK and allowing CMake to automatically locate the LAPACK library, it is not necessary to also enable BLAS as CMake will find the corresponding BLAS library and include it when searching for LAPACK.



### 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 are 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 NVIDIA website: <https://developer.nvidia.com/cuda-downloads>. To enable CUDA, set `CUDA_ENABLE` to `ON`. If you installed CUDA 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

To build SUNDIALS RAJA modules you need to enable SUNDIALS CUDA support, first. You also need a CUDA-enabled RAJA installation on your system. RAJA is free software, developed by Lawrence Livermore National Laboratory, and can be obtained from <https://github.com/LLNL/RAJA>. Next you need to set `RAJA_ENABLE` to `ON`, to enable building the RAJA vector module, and `EXAMPLES_ENABLE_RAJA` to `ON` to build the RAJA examples. If you installed RAJA to a nonstandard location you will be prompted to set the variable `RAJA_DIR` with the path to the RAJA CMake configuration file. SUNDIALS was tested with RAJA version 0.3.

## 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 *srcdir*
2. Create a separate *builddir*
3. Open a Visual Studio Command Prompt and `cd` to *builddir*
4. Run `cmake-gui ../srcdir`
  - (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           | sundials/sundials_fconfig.h  |
|                        |              | sundials/sundials_types.h            | sundials/sundials_math.h     |
|                        |              | sundials/sundials_nvector.h          | sundials/sundials_fnvector.h |
|                        |              | sundials/sundials_iterative.h        | sundials/sundials_direct.h   |
|                        |              | sundials/sundials_dense.h            | sundials/sundials_band.h     |
|                        |              | sundials/sundials_matrix.h           | 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               |                              |
|                        |              | nvector/cuda/ThreadPartitioning.hpp  |                              |
|                        |              | nvector/cuda/Vector.hpp              |                              |
|                        |              | nvector/cuda/VectorKernels.cuh       |                              |
| continued on next page |              |                                      |                              |

|                                 |              |   |
|---------------------------------|--------------|---|
| <i>continued from last page</i> |              |   |
| 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   |
| 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_SPFGMR                | Libraries    | libsundials_sunlinsolspfgmr. <i>lib</i><br>libsundials_fsunlinsolspfgmr.a           |
|                                 | Header files | sunlinsol/sunlinsol_spfgmr.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         |
|                                 |              |   |
| <i>continued on next page</i>   |              |   |

|                                 |              |   |                        |
|---------------------------------|--------------|---|------------------------|
| <i>continued from last page</i> |              |   |                        |
|                                 | Header files | sunlinsol/sunlinsol_sptfqmr.h   |                        |
| SUNLINSOL_SUPERLUMT             | Libraries    | libsundials_sunlinsolsuperlumt. <i>lib</i><br>libsundials_fsunlinsolsuperlumt.a |                        |
|                                 | Header files | sunlinsol/sunlinsol_superlumt.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  |
|                                 |              | arkode/arkode_bandpre.h   | arkode/arkode_bbdpre.h |
| IDA                             | Libraries    | libsundials_ida. <i>lib</i>   | libsundials_fida.a     |
|                                 | Header files | ida/ida.h   | ida/ida_impl.h         |
|                                 |              | ida/ida_direct.h  | ida/ida_spils.h        |
|                                 |              | ida/ida_bbdpre.h  |                        |
| IDAS                            | Libraries    | libsundials_idas. <i>lib</i>  |                        |
|                                 | Header files | idas/idas.h   | idas/idas_impl.h       |
|                                 |              | idas/idas_direct.h  | idas/idas_spils.h      |
|                                 |              | idas/idas_bbdpre.h  |                        |
| KINSOL                          | Libraries    | libsundials_kinsol. <i>lib</i>  | libsundials_fkinsol.a  |
|                                 | Header files | kinsol/kinsol.h   | kinsol/kinsol_impl.h   |
|                                 |              | kinsol/kinsol_direct.h  | kinsol/kinsol_spils.h  |
|                                 |              | kinsol/kinsol_bbdpre.h  |                        |

# Appendix B

## CVODES Constants

Below we list all input and output constants used by the main solver and linear solver modules, together with their numerical values and a short description of their meaning.

### B.1 CVODES input constants

| CVODES <b>main solver module</b>    |   |   |
|-------------------------------------|---|---|
| CV_ADAMS                            | 1 | Adams-Moulton linear multistep method.  |
| CV_BDF                              | 2 | BDF linear multistep method.  |
| CV_FUNCTIONAL                       | 1 | Nonlinear system solution through functional iterations.                            |
| CV_NEWTON                           | 2 | Nonlinear system solution through Newton iterations.                                |
| CV_NORMAL                           | 1 | Solver returns at specified output time.  |
| CV_ONE_STEP                         | 2 | Solver returns after each successful step.  |
| CV_SIMULTANEOUS                     | 1 | Simultaneous corrector forward sensitivity method.                                  |
| CV_STAGGERED                        | 2 | Staggered corrector forward sensitivity method.                                     |
| CV_STAGGERED1                       | 3 | Staggered (variant) corrector forward sensitivity method.                           |
| CV_CENTERED                         | 1 | Central difference quotient approximation ( $2^{nd}$ order) of the sensitivity RHS. |
| CV_FORWARD                          | 2 | Forward difference quotient approximation ( $1^{st}$ order) of the sensitivity RHS. |
| CVODES <b>adjoint solver module</b> |   |   |
| CV_HERMITE                          | 1 | Use Hermite interpolation.  |
| CV_POLYNOMIAL                       | 2 | Use variable-degree polynomial interpolation.                                       |
| 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 CVODES output constants

| CVODES <b>main solver module</b> |     |   |
|----------------------------------|-----|---|
| 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 <b>mxstep</b> 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 <b>cvode_mem</b> 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 <b>CVodeMalloc</b> .  |
| CV_BAD_K                         | -24 | The derivative order $k$ is larger than the order used.   |
| CV_BAD_T                         | -25 | The time $t$ is outside the last step taken.  |
| CV_BAD_DKY                       | -26 | The output derivative vector is NULL.   |
| CV_TOO_CLOSE                     | -27 | The output and initial times are too close to each other.   |
| CV_NO_QUAD                       | -30 | Quadrature integration was not activated.   |
| CV_QRHSFUNC_FAIL                 | -31 | The quadrature right-hand side function failed in an unrecoverable manner.  |



|                        |     |  |
|------------------------|-----|--|
| CV_FIRST_QRHSFUNC_ERR  | -32 | The quadrature right-hand side function failed at the first call.                              |
| CV_REPTD_QRHSFUNC_ERR  | -33 | The quadrature right-hand side function had repeated recoverable errors.                       |
| CV_UNREC_QRHSFUNC_ERR  | -34 | The quadrature right-hand side function had a recoverable error, but no recovery is possible.  |
| CV_NO_SENS             | -40 | Forward sensitivity integration was not activated.   |
| CV_SRHSFUNC_FAIL       | -41 | The sensitivity right-hand side function failed in an unrecoverable manner.                    |
| CV_FIRST_SRHSFUNC_ERR  | -42 | The sensitivity right-hand side function failed at the first call.                             |
| CV_REPTD_SRHSFUNC_ERR  | -43 | The sensitivity right-hand side function had repeated recoverable errors.                      |
| CV_UNREC_SRHSFUNC_ERR  | -44 | The sensitivity right-hand side function had a recoverable error, but no recovery is possible. |
| CV_BAD_IS              | -45 | The sensitivity index is larger than the number of sensitivities computed.                     |
| CV_NO_QUADSENS         | -50 | Forward sensitivity integration was not activated.   |
| CV_QSRHSFUNC_FAIL      | -51 | The sensitivity right-hand side function failed in an unrecoverable manner.                    |
| CV_FIRST_QSRHSFUNC_ERR | -52 | The sensitivity right-hand side function failed at the first call.                             |
| CV_REPTD_QSRHSFUNC_ERR | -53 | The sensitivity right-hand side function had repeated recoverable errors.                      |
| CV_UNREC_QSRHSFUNC_ERR | -54 | The sensitivity right-hand side function had a recoverable error, but no recovery is possible. |

---

**CVODES adjoint solver module**


---

|                |      |   |
|----------------|------|---|
| CV_NO_ADJ      | -101 | Adjoint module was not initialized.   |
| CV_NO_FWD      | -102 | The forward integration was not yet performed.  |
| CV_NO_BCK      | -103 | No backward problem was specified.  |
| CV_BAD_TBO     | -104 | The final time for the adjoint problem is outside the interval over which the forward problem was solved. |
| CV_REIFWD_FAIL | -105 | Reinitialization of the forward problem failed at the first checkpoint.                                   |
| CV_FWD_FAIL    | -106 | An error occurred during the integration of the forward problem.  |
| CV_GETY_BADT   | -107 | Wrong time in interpolation function.   |

---

**CVDLS linear solver modules**


---

|                 |    |   |
|-----------------|----|---|
| CVDLS_SUCCESS   | 0  | Successful function return.   |
| CVDLS_MEM_NULL  | -1 | The <code>cvode_mem</code> argument was NULL.                       |
| CVDLS_LMEM_NULL | -2 | The CVDLS linear solver has not been initialized.                   |
| CVDLS_ILL_INPUT | -3 | The CVDLS solver is not compatible with the current NVECTOR module. |

|  |      |  |
|--|------|--|
| CVDLS_MEM_FAIL                                   | -4   | A memory allocation request failed.  |
| CVDLS_JACFUNC_UNRECVR                            | -5   | The Jacobian function failed in an unrecoverable manner.   |
| CVDLS_JACFUNC_RECVR                              | -6   | The Jacobian function had a recoverable error.   |
| CVDLS_SUNMAT_FAIL                                | -7   | An error occurred with the current SUNMATRIX module.   |
| CVDLS_NO_ADJ                                     | -101 | The combined forward-backward problem has not been initialized.                                      |
| CVDLS_LMEMB_NULL                                 | -102 | The linear solver was not initialized for the backward phase.  |
| <hr/> <b>CVDIAG linear solver module</b> <hr/>   |      |  |
| 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.  |
| CVDIAG_NO_ADJ                                    | -101 | The combined forward-backward problem has not been initialized.                                      |
| <hr/> <b>CVSPILS linear solver modules</b> <hr/> |      |  |
| 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.   |
| CVSPILS_NO_ADJ                                   | -101 | The combined forward-backward problem has not been initialized.                                      |
| CVSPILS_LMEMB_NULL                               | -102 | The linear solver was not initialized for the backward phase.  |

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