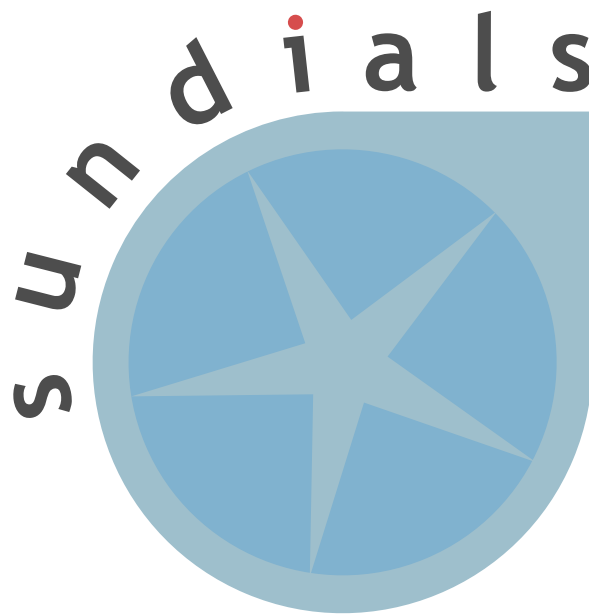


# User Documentation for CVODE v2.9.0 (SUNDIALS v2.7.0)

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# Chapter 1

## Introduction

CVODE is part of a software family called SUNDIALS: SUite of Nonlinear and Differential/ALgebraic equation Solvers [18]. This suite consists of CVODE, ARKODE, KINSOL, and IDA, and variants of these with sensitivity analysis capabilities.

### 1.1 Historical Background

FORTRAN solvers for ODE initial value problems are widespread and heavily used. Two solvers that have been written at LLNL in the past are VODE [3] and VODPK [5]. VODE is a general purpose solver that includes methods for 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 [24]. 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 contains three Krylov methods that can be used in conjunction with Newton iteration: the GMRES (Generalized Minimal RESidual) [26], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [27], and TFQMR (Transpose-Free Quasi-Minimal Residual) linear iterative methods [13]. 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 three Krylov methods in CVODE, we recommend GMRES as the best overall choice. However, users are encouraged to compare all three, 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.

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 [8], the parallel variant of CVODE.

Recently, the functionality of CVODE and PVODE has been combined into one single code, simply called CVODE. Development of the new version of CVODE was concurrent with a redesign of the vector operations module across the SUNDIALS suite. The key feature of the NVECTOR module is that it is written in terms of abstract vector operations with the actual vector kernels attached by a particular

implementation (such as serial or parallel) of NVECTOR. This allows writing the SUNDIALS solvers in a manner independent of the actual NVECTOR implementation (which can be user-supplied), as well as allowing more than one NVECTOR module linked into an executable file. SUNDIALS (and thus CVODE) is supplied with six different NVECTOR implementations: serial, MPI-parallel, and both openMP and Pthreads thread-parallel NVECTOR implementations, a Hypre parallel implementation, and a PetSC implementation.

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

## 1.2 Changes from previous versions

### Changes in v2.9.0

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

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

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

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

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

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

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

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

### Changes in v2.8.0

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

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

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

In `CVLapackBand`, the line `smu = MIN(N-1,mu+m1)` was changed to `smu = mu + m1` to correct an illegal input error for DGBTRF/DGBTRS.

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

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

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

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

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

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

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

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

## Changes in v2.7.0

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

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

## Changes in v2.6.0

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

The user interface has been further refined. Some of the API changes involve: (a) a reorganization of all linear solver modules into two families (besides the existing family of scaled preconditioned iterative linear solvers, the direct solvers, including the new Lapack-based ones, were also organized into a *direct* family); (b) maintaining a single pointer to user data, optionally specified through a `Set-type` function; and (c) a general streamlining of the preconditioner modules distributed with the solver.

## Changes in v2.5.0

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

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

## Changes in v2.4.0

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

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

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

## Changes in v2.3.0

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

## Changes in v2.2.1

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

## Changes in v2.2.0

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

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

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

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

## 1.3 Reading this User Guide

This user guide is a combination of general usage instructions and specific example programs. We expect that some readers will want to concentrate on the general instructions, while others will refer

mostly to the examples, and the organization is intended to accommodate both styles.

There are different possible levels of usage of CVODE. The most casual user, with a small IVP problem only, can get by with reading §2.1, then Chapter 4 through §4.5.5 only, and looking at examples in [19]. In a different direction, a more expert user with an IVP problem may want to (a) use a package preconditioner (§4.7), (b) supply his/her own Jacobian or preconditioner routines (§4.6), (c) do multiple runs of problems of the same size (§4.5.9), (d) supply a new NVECTOR module (Chapter 6), or even (e) supply a different linear solver module (§3.2 and Chapter 7).

The structure of this document is as follows:

- In Chapter 2, we give short descriptions of the numerical methods implemented by CVODE for the solution of initial value problems for systems of ODEs, and continue with short descriptions of preconditioning (§2.2), stability limit detection (§2.3), and rootfinding (§2.4).
- The following chapter describes the structure of the SUNDIALS suite of solvers (§3.1) and the software organization of the CVODE solver (§3.2).
- Chapter 4 is the main usage document for CVODE for C applications. It includes a complete description of the user interface for the integration of ODE initial value problems.
- In Chapter 5, we describe FCVODE, an interface module for the use of CVODE with FORTRAN applications.
- Chapter 6 gives a brief overview of the generic NVECTOR module shared among the various components of SUNDIALS, and details on the NVECTOR implementations provided with SUNDIALS: a serial implementation (§6.1), a distributed memory parallel implementation based on MPI (§6.2), and two thread-parallel implementations based on openMP (§6.3) and Pthreads (§6.4), respectively.
- Chapter 7 describes the interfaces to the linear solver modules, so that a user can provide his/her own such module.
- Chapter 8 describes in detail the generic linear solvers shared by all SUNDIALS solvers.
- Finally, in the appendices, we provide detailed instructions for the installation of CVODE, within the structure of SUNDIALS (Appendix A), as well as a list of all the constants used for input to and output from CVODE functions (Appendix B).

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



**Acknowledgments.** We wish to acknowledge the contributions to previous versions of the CVODE and PVODE codes and their user guides by Scott D. Cohen [9] and George D. Byrne [7].

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## Chapter 2

# Mathematical Considerations

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

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

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

### 2.1 IVP solution

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

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

Here the  $y^n$  are computed approximations to  $y(t_n)$ , and  $h_n = t_n - t_{n-1}$  is the step size. The user of CVODE must choose appropriately one of two multistep methods. For nonstiff problems, CVODE includes the Adams-Moulton formulas, characterized by  $K_1 = 1$  and  $K_2 = q$  above, where the order  $q$  varies between 1 and 12. For stiff problems, CVODE includes the Backward Differentiation Formulas (BDFs) in so-called fixed-leading coefficient 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 [22].

For either choice of formula, the nonlinear system

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

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, CVODE 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

$$M[y^{n(m+1)} - y^{n(m)}] = -G(y^{n(m)}), \quad (2.4)$$

in which

$$M \approx I - \gamma J, \quad J = \partial f / \partial y, \quad \text{and} \quad \gamma = h_n \beta_{n,0}. \quad (2.5)$$

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, CVODE provides several choices, including the option of an user-supplied linear solver module. The linear solver modules distributed with SUNDIALS are organized in three families, a *direct* family comprising direct linear solvers for dense or banded matrices, a *sparse* family comprising direct linear solvers for matrices stored in compressed-sparse-column format, and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. In addition, CVODE also provides a linear solver module which only uses a diagonal approximation of the Jacobian matrix. 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 [23, 12, 2] (serial or threaded vector modules only) [Note that users will need to download and install the KLU or SuperLU\_MT packages independent of CVODE],
- a diagonal approximate Jacobian solver,
- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver without restarts,
- SPBCG, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver, or
- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver.

For large stiff systems, where direct methods are not feasible, the combination of a BDF integrator and any of the preconditioned Krylov methods (SPGMR, SPBCG, or SPTFQMR) 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]. Note that the direct linear solvers (dense, band and sparse) can only be used with the serial and threaded vector representations.

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

$$W_i = 1/[\text{RTOL} \cdot |y_i| + \text{ATOL}_i]. \quad (2.6)$$

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 (2.3), we want to ensure that the iteration error  $y^n - y^{n(m)}$  is small relative to  $\epsilon$ , specifically that it is less than  $0.1\epsilon$ . (The safety factor 0.1 can be changed by the user.) For this, we also estimate the linear convergence rate constant  $R$  as follows. We initialize  $R$  to 1, and reset  $R = 1$  when  $M$  or  $P$  is updated. After computing a correction  $\delta_m = y^{n(m)} - y^{n(m-1)}$ , we update  $R$  if  $m > 1$  as

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

Now we use the estimate

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

Therefore the convergence (stopping) test is

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

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

When a Krylov method is used to solve the linear system, its errors must also be controlled, and this also involves the local error test constant. The linear iteration error in the solution vector  $\delta_m$  is approximated by the preconditioned residual vector. Thus to ensure (or attempt to ensure) that the linear iteration errors do not interfere with the nonlinear error and local integration error controls, we require that the norm of the preconditioned residual be less than  $0.05 \cdot (0.1\epsilon)$ .

With the direct dense and band methods, the Jacobian may be supplied by a user routine, or approximated by difference quotients, at the user's option. In the latter case, we use the usual approximation

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

The increments  $\sigma_j$  are given by

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

where  $U$  is the unit roundoff,  $\sigma_0$  is a dimensionless value, and  $W_j$  is the error weight defined in (2.6). 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 compressed-sparse-column format.

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

$$Jv = [f(t, y + \sigma v) - f(t, y)]/\sigma. \quad (2.7)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

and

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

The new order and step size are then set according to

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

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

The various algorithmic features of CVODE described above, as inherited from the solvers VODE and VODPK, are documented in [3, 5, 17]. They are also summarized in [18].

Normally, CVODE takes steps until a user-defined output value  $t = t_{\text{out}}$  is overtaken, and then it computes  $y(t_{\text{out}})$  by interpolation. However, a “one step” mode option is available, where control returns to the calling program after each step. There are also options to force CVODE not to integrate past a given stopping point  $t = t_{\text{stop}}$ .

## 2.2 Preconditioning

When using a Newton method to solve the nonlinear system (2.3), CVODE makes repeated use of a linear solver to solve linear systems of the form  $Mx = -r$ , where  $x$  is a correction vector and  $r$  is a residual vector. If this linear system solve is done with one of the scaled preconditioned iterative linear solvers, these solvers are rarely successful if used without preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system  $Ax = b$  can be preconditioned on the left, as  $(P^{-1}A)x = P^{-1}b$ ; on the right, as  $(AP^{-1})Px = b$ ; or on both sides, as  $(P_L^{-1}AP_R^{-1})P_Rx = P_L^{-1}b$ . The Krylov method is then applied to a system with the matrix  $P^{-1}A$ , or  $AP^{-1}$ , or  $P_L^{-1}AP_R^{-1}$ , instead of  $A$ . In order to improve the convergence of the Krylov iteration, the preconditioner matrix  $P$ , or the product  $P_LP_R$  in the last case, should in some sense approximate the system matrix  $A$ . Yet at the same time, in order to be cost-effective, the matrix  $P$ , or matrices  $P_L$  and  $P_R$ , should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [4] for an extensive study of preconditioners for reaction-transport systems).

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

Typical preconditioners used with CVODE are based on approximations to the system Jacobian,  $J = \partial f / \partial y$ . Since the 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

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

When the BDF option is selected, CVODE 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 in 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 [15]. The algorithm supplements (but differs greatly from) the existing algorithms in CVODE for choosing step size and order based on estimated local truncation errors. It works directly with history data that is readily available in CVODE. If it concludes that the step size is in fact stability-limited, it dictates a reduction in the method order, regardless of the outcome of the error-based algorithm. The STALD algorithm has been tested in combination with the VODE solver on linear advection-dominated advection-diffusion problems [16], where it works well. The implementation in CVODE has been successfully tested on linear and nonlinear advection-diffusion problems, among others.

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

## 2.4 Rootfinding

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

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

The basic scheme used is to check for sign changes of any  $g_i(t)$  over each time step taken, and then (when a sign change is found) to home in on the root (or roots) with a modified secant method [14].

In addition, each time  $g$  is computed, CVODE checks to see if  $g_i(t) = 0$  exactly, and if so it reports this as a root. However, if an exact zero of any  $g_i$  is found at a point  $t$ , CVODE computes  $g$  at  $t + \delta$  for a small increment  $\delta$ , slightly further in the direction of integration, and if any  $g_i(t + \delta) = 0$  also, CVODE stops and reports an error. This way, each time CVODE takes a time step, it is guaranteed that the values of all  $g_i$  are nonzero at some past value of  $t$ , beyond which a search for roots is to be done.

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

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

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

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

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

where  $\alpha$  a weight parameter. On the first two passes through the loop,  $\alpha$  is set to 1, making  $t_{mid}$  the secant method value. Thereafter,  $\alpha$  is reset according to the side of the subinterval (low vs high, i.e. toward  $t_{lo}$  vs toward  $t_{hi}$ ) in which the sign change was found in the previous two passes. If the two sides were opposite,  $\alpha$  is set to 1. If the two sides were the same,  $\alpha$  is halved (if on the low side) or doubled (if on the high side). The value of  $t_{mid}$  is closer to  $t_{lo}$  when  $\alpha < 1$  and closer to  $t_{hi}$  when  $\alpha > 1$ . If the above value of  $t_{mid}$  is within  $\tau/2$  of  $t_{lo}$  or  $t_{hi}$ , it is adjusted inward, such that its fractional distance from the endpoint (relative to the interval size) is between .1 and .5 (.5 being the midpoint), and the actual distance from the endpoint is at least  $\tau/2$ .



## Chapter 3

# Code Organization

### 3.1 SUNDIALS organization

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

The various solvers of this family share many subordinate modules. For this reason, it is organized as a family, with a directory structure that exploits that sharing (see 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  $Mdy/dt = f(t, y)$  based on additive Runge-Kutta methods;
- IDA, a solver for differential-algebraic systems  $F(t, y, \dot{y}) = 0$  based on BDF methods;
- IDAS, a solver for differential-algebraic systems with sensitivity analysis capabilities;
- KINSOL, a solver for nonlinear algebraic systems  $F(u) = 0$ .

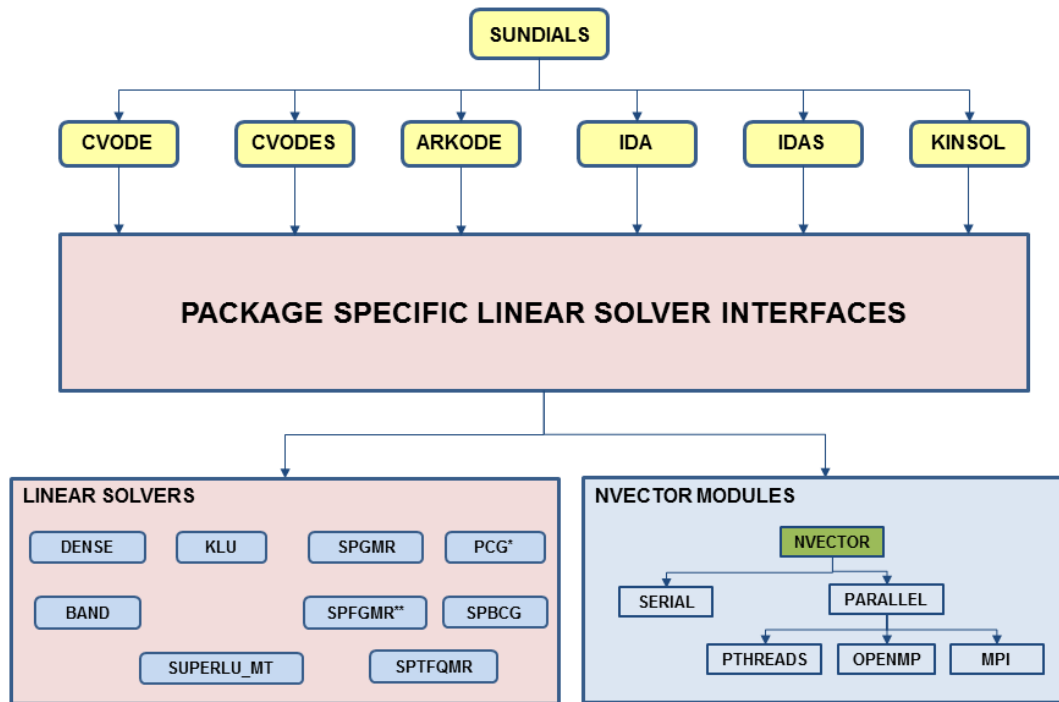
### 3.2 CVODE organization

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

The overall organization of the CVODE package is shown in Figure 3.2. 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 modules is specified, and is then invoked as needed during the integration.

At present, the package includes the following eight CVODE linear algebra modules, organized into two families. The *direct* family of linear solvers provides solvers for the direct solution of linear systems with dense, banded, or sparse matrices, and includes:

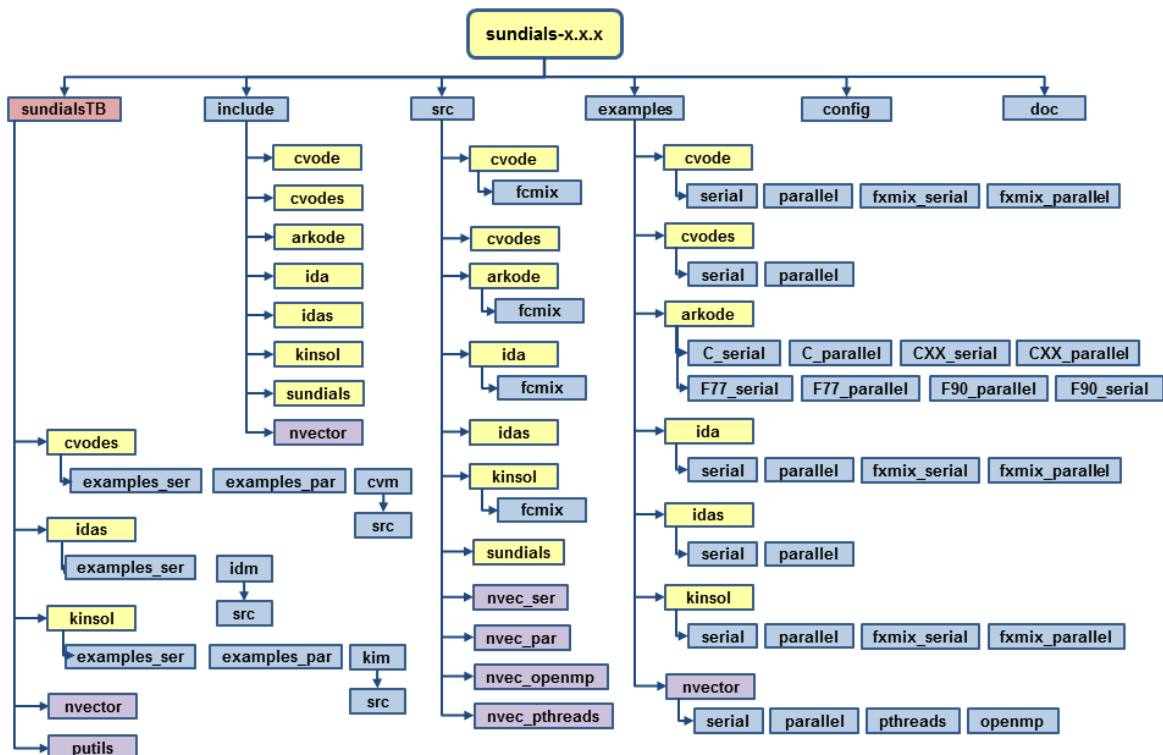
- CVDENSE: LU factorization and backsolving with dense matrices (using either an internal implementation or Blas/Lapack);



(a) High-level diagram (note that none of the Lapack-based linear solver modules are represented.)

\* only applies to ARKODE

\*\* only applies to ARKODE and KINSOL



(b) Directory structure of the source tree

Figure 3.1: Organization of the SUNDIALS suite

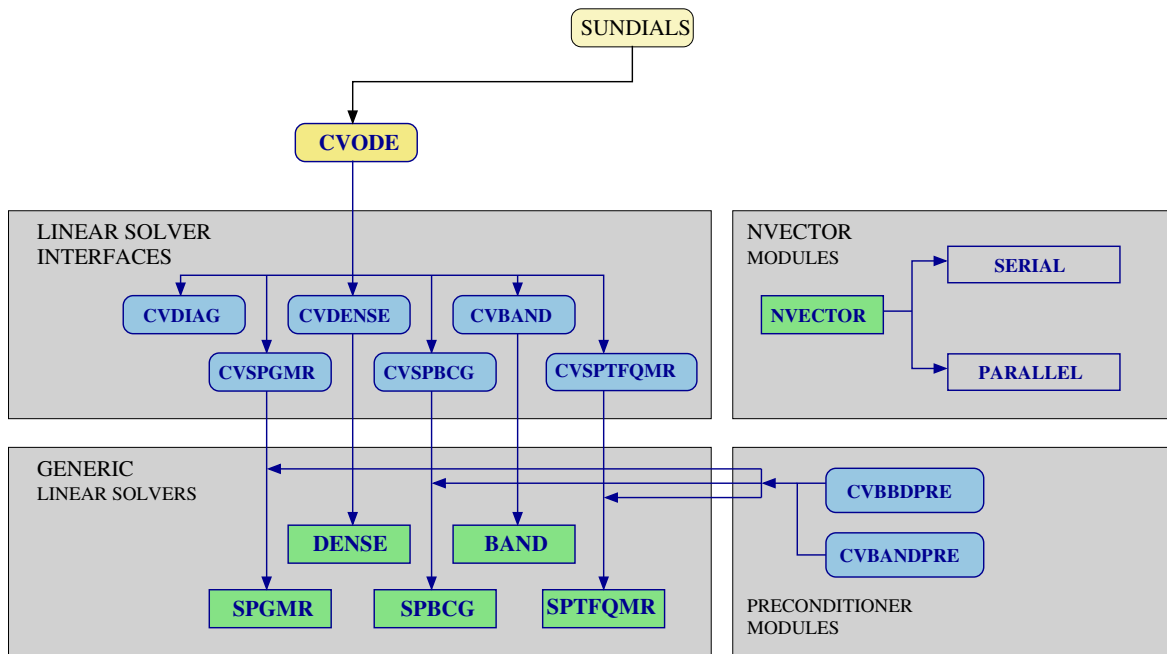


Figure 3.2: Overall structure diagram of the CVODE package. Modules specific to CVODE are distinguished by rounded boxes, while generic solver and auxiliary modules are in rectangular boxes. Note that the direct linear solvers using Lapack implementations are not explicitly represented. Note also that the KLU and SuperLU\_MT support is through interfaces to packages. Users will need to download and compile those packages independently.

- CVBAND: LU factorization and backsolving with banded matrices (using either an internal implementation or Blas/Lapack);
- CVKLU: LU factorization and backsolving with compressed-sparse-column (CSC) matrices using the KLU linear solver library [11, 1] (KLU to be downloaded and compiled by user independent of CVODE);
- CVSUPERLUMT: LU factorization and backsolving with compressed-sparse-column (CSC) matrices using the threaded SuperLU\_MT linear solver library [23, 12, 2] (SuperLU\_MT to be downloaded and compiled by user independent of CVODE).

The *spils* family of linear solvers provides scaled preconditioned iterative linear solvers and includes:

- CVSPGMR: scaled preconditioned GMRES method;
- CVSPBCG: scaled preconditioned Bi-CGStab method;
- CVSPTFQMR: scaled preconditioned TFQMR method.

Additionally, CVODE includes:

- CVDIAG: an internally generated diagonal approximation to the Jacobian;

The set of linear solver modules distributed with CVODE is intended to be expanded in the future as new algorithms are developed. Note that users wishing to employ KLU or SuperLU\_MT will need to download and install these libraries independent of SUNDIALS. SUNDIALS provides only the interfaces between itself and these libraries.

In the case of the direct methods CVDENSE and CVBAND the package includes an algorithm for the approximation of the Jacobian by difference quotients, but the user also has the option of supplying

the Jacobian (or an approximation to it) directly. When using the sparse direct linear solvers CVKLU and CVSUPERLUMT, the user must supply a routine for the Jacobian (or an approximation to it) in CSC format, since standard difference quotient approximations do not leverage the inherent sparsity of the problem. In the case of the Krylov iterative methods CVSPGMR, CVSPBCG, and CVSPTFQMR, the package includes an algorithm for the approximation by difference quotients of the product between the Jacobian matrix and a vector of appropriate length. Again, the user has the option of providing a routine for this operation. For the Krylov methods, the preconditioning must be supplied by the user, in two phases: setup (preprocessing of Jacobian data) 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 CVODE, offer considerable assistance in building preconditioners.

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

These modules are also decomposed in another way. With the exception of CVDIAG, each of the linear solver modules (CVDENSE etc.) consists of an interface built on top of a generic linear system solver (DENSE etc.). The interface deals with the use of the particular method in the CVODE context, whereas the generic solver is independent of the context. While some of the generic linear system solvers (DENSE, BAND, SPGMR, SPBCG, and SPTFQMR) were written with SUNDIALS in mind, they are intended to be usable anywhere as general-purpose solvers. This separation also allows for any generic solver to be replaced by an improved version, with no necessity to revise the CVODE package elsewhere.

CVODE also provides two preconditioner modules, for use with any of the Krylov iterative linear solvers. The first one, CVBANDPRE, is intended to be used with NVECTOR\_SERIAL, NVECTOR\_OPENMP or NVECTOR\_PTHREADS and provides a banded difference-quotient Jacobian-based preconditioner, with corresponding setup and solve routines. The second preconditioner module, CVBBDPRE, works in conjunction with NVECTOR\_PARALLEL and generates a preconditioner that is a block-diagonal matrix with each block being a band matrix.

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

## Chapter 4

# Using CVODE for C Applications

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

The sample programs described in the companion document [19] may also be helpful. Those codes may be used as templates (with the removal of some lines used in testing) and are included in the CVODE package.

Users with applications written in FORTRAN77 should see Chapter 5, which describes the FORTRAN/C interface module.

The user should be aware that not all linear solver modules are compatible with all NVECTOR implementations. For example, NVECTOR\_PARALLEL is not compatible with the direct dense, direct band or direct sparse linear solvers since these linear solver modules need to form the complete system Jacobian. The following CVODE modules can only be used with either NVECTOR\_SERIAL, NVECTOR\_OPENMP or NVECTOR\_PTHREADS: CVDENSE, CVBAND (using either the internal or the Lapack implementation), CVKLU, CVSUPERLUMT and CVBANDPRE. 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. Also, the preconditioner module CVBBDPRE can only be used with NVECTOR\_PARALLEL.

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

### 4.1 Access to library and header files

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

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

- *libdir/libsundials\_cvode.lib*,
- *libdir/libsundials\_nvec\*.lib* (one to four files),

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

- *incdir/include/cvode*
- *incdir/include/sundials*
- *incdir/include/nvector*

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

## 4.2 Data Types

The `sundials_types.h` file contains the definition of the type `realtype`, which is used by the SUNDIALS solvers for all floating-point data. The 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).

## 4.3 Header files

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

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

Note that `cvode.h` includes `sundials_types.h`, which defines the types `realtype` and `booleantype` and the constants `FALSE` and `TRUE`.

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

Finally, 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 solvers available for use with CVODE are:

- `cvode_dense.h`, which is used with the dense direct linear solver;
- `cvode_band.h`, which is used with the band direct linear solver;
- `cvode_lapack.h`, which is used with Lapack implementations of dense or band direct linear solvers;
- `cvode_diag.h`, which is used with the diagonal linear solver;
- `cvode_klu.h`, which is used with the KLU sparse direct linear solver;

- `cvode_superlunt.h`, which is used with the SuperLU-MT threaded sparse direct linear solver;
- `cvode_spgmr.h`, which is used with the scaled, preconditioned GMRES Krylov linear solver SPGMR;
- `cvode_spgbcs.h`, which is used with the scaled, preconditioned Bi-CGStab Krylov linear solver SPBCG;
- `cvode_sptfqmr.h`, which is used with the scaled, preconditioned TFQMR Krylov solver SPT-FQMR;

The header files for the dense and banded linear solvers (both internal and Lapack) include the file `cvode_direct.h`, which defines common functions. This in turn includes a file (`sundials_direct.h`) which defines the matrix type for these direct linear solvers (`DlsMat`), as well as various functions and macros acting on such matrices.

The header files for the KLU and SuperLU-MT sparse linear solvers include the file `cvode_sparse.h`, which defines common functions. This in turn includes a file (`sundials_sparse.h`) which defines the matrix type for these sparse direct linear solvers (`SlsMat`), as well as various functions and macros acting on such matrices.

The header files for the Krylov iterative solvers include `cvode_spils.h` which defines common functions and which in turn includes a header file (`sundials_iterative.h`) which enumerates the kind of preconditioning and (for the SPGMR solver only) the choices for the Gram-Schmidt process.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the `cvDiurnal_kry_p` example (see [19]), preconditioning is done with a block-diagonal matrix. For this, even though the CVSPGMR linear solver is used, the header `sundials_dense.h` is included for access to the underlying generic dense linear solver.

## 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 implementation used. For the steps that are not, refer to Chapter 6 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 `long int`.

### 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, use a call of the form `y0 = N_VMake_***(..., ydata)` if the `realtype` array `ydata` containing the initial values of `y` already exists. Otherwise, create a new vector by making a call of the form `y0 = N_VNew_***(...)`, and then set its elements by accessing the underlying data with a call of the form `ydata = N_VGetArrayPointer_***(y0)`. See §6.1-6.4 for details.

For the *hypr* and PETSc vector wrappers, first create and initialize the underlying vector, and then create 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 §6.5 and §6.6 for details.

#### 4. Create CVODE object

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

#### 5. Initialize CVODE solver

Call `CVodeInit(...)` to provide required problem specifications, allocate internal memory for CVODE, and initialize CVODE. `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 CVODE from their default values. See §4.5.6.1 for details.

#### 8. Attach linear solver module

If Newton iteration is chosen, initialize the linear solver module with one of the following calls (for details see §4.5.3):

```
ier = CVDense(...);
ier = CVBand(...);
ier = CVLapackDense(...);
ier = CVLapackBand(...);
ier = CVKLU(...);
ier = CVSuperLUMT(...);
ier = CVDiag(...);
ier = CVSpqr(...);
ier = CVSpbcg(...);
ier = CVSptfqmr(...);
```

NOTE: The direct (dense or band) and sparse linear solver options are usable only in a serial environment.

#### 9. Set linear solver optional inputs

Call `CV*Set*` functions from the selected linear solver module to change optional inputs specific to that linear solver. See §4.5.6 for details.

#### 10. 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 §4.5.6.5 for relevant optional input calls.

#### 11. 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.

**12. Get optional outputs**

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

**13. 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);
```

**14. Free solver memory**

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

**15. 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 in SUNDIALS packages and the vector implementations required for use. As an example, one cannot use the SUNDIALS package specific dense direct solver interfaces with the MPI-based vector implementation. However, as discussed in Chapter 8 the direct dense, direct band, and iterative spils solvers provided with SUNDIALS are written in a way that allows a user to develop their own solvers around them should a user so desire.

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

Linear Solver Interface	Serial	Parallel (MPI)	OpenMP	pThreads	hypre Vector	PETSc Vector	User Supplied
Dense	✓		✓	✓			✓
Band	✓		✓	✓			✓
LapackDense	✓		✓	✓			✓
LapackBand	✓		✓	✓			✓
KLU	✓		✓	✓			✓
SUPERLUMT	✓		✓	✓			✓
SPGMR	✓	✓	✓	✓	✓	✓	✓
SPFGMR	✓	✓	✓	✓	✓	✓	✓
SPBCG	✓	✓	✓	✓	✓	✓	✓
SPTFQMR	✓	✓	✓	✓	✓	✓	✓
User supplied	✓	✓	✓	✓	✓	✓	✓

## 4.5 User-callable functions

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

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

### 4.5.1 CVODE initialization and deallocation functions

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

#### CVodeCreate

Call	<code>cvode_mem = CVodeCreate(lmm, iter);</code>
Description	The function <code>CVodeCreate</code> instantiates a CVODE solver object and specifies the solution method.
Arguments	<p><code>lmm</code> (<code>int</code>) 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>iter</code> (<code>int</code>) specifies the type of nonlinear solver iteration and may be either <code>CV_NEWTON</code> or <code>CV_FUNCTIONAL</code>.</p> <p>The recommended choices for (<code>lmm</code>, <code>iter</code>) are (<code>CV_ADAMS</code>, <code>CV_FUNCTIONAL</code>) for nonstiff problems and (<code>CV_BDF</code>, <code>CV_NEWTON</code>) for stiff problems.</p>
Return value	If successful, <code>CVodeCreate</code> returns a pointer to the newly created CVODE memory block (of type <code>void *</code> ). Otherwise, it returns <code>NULL</code> .

#### CVodeInit

Call	<code>flag = CVodeInit(cvode_mem, f, t0, y0);</code>
Description	The function <code>CVodeInit</code> provides required problem and solution specifications, allocates internal memory, and initializes CVODE.
Arguments	<p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block returned by <code>CVodeCreate</code>.</p> <p><code>f</code> (<code>CVRhsFn</code>) is the C function which computes the right-hand side function <math>f</math> in the ODE. This function has the form <code>f(t, y, ydot, user_data)</code> (for full details see §4.6.1).</p> <p><code>t0</code> (<code>realtype</code>) is the initial value of <math>t</math>.</p> <p><code>y0</code> (<code>N_Vector</code>) is the initial value of <math>y</math>.</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>CVodeInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The CVODE 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>CVodeInit</code> has an illegal value.</p>
Notes	If an error occurred, <code>CVodeInit</code> also sends an error message to the error handler function.

#### CVodeFree

Call	<code>CVodeFree(&amp;cvode_mem);</code>
Description	The function <code>CVodeFree</code> frees the memory allocated by a previous call to <code>CVodeCreate</code> .
Arguments	The argument is the pointer to the CVODE memory block (of type <code>void *</code> ).
Return value	The function <code>CVodeFree</code> has no return value.

### 4.5.2 CVODE tolerance specification functions

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

**CVodeSStolerances**

Call	<code>flag = CVodeSStolerances(cvode_mem, reltol, abstol);</code>
Description	The function <code>CVodeSStolerances</code> specifies scalar relative and absolute tolerances.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block returned by <code>CVodeCreate</code> . <code>reltol</code> ( <code>realtype</code> ) is the scalar relative error tolerance. <code>abstol</code> ( <code>realtype</code> ) is the scalar absolute error tolerance.
Return value	The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <code>CV_SUCCESS</code> The call to <code>CVodeSStolerances</code> was successful. <code>CV_MEM_NULL</code> The CVODE memory block was not initialized through a previous call to <code>CVodeCreate</code> . <code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called. <code>CV_ILL_INPUT</code> One of the input tolerances was negative.

**CVodeSVtolerances**

Call	<code>flag = CVodeSVtolerances(cvode_mem, reltol, abstol);</code>
Description	The function <code>CVodeSVtolerances</code> specifies scalar relative tolerance and vector absolute tolerances.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block returned by <code>CVodeCreate</code> . <code>reltol</code> ( <code>realtype</code> ) is the scalar relative error tolerance. <code>abstol</code> ( <code>N_Vector</code> ) is the vector of absolute error tolerances.
Return value	The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <code>CV_SUCCESS</code> The call to <code>CVodeSVtolerances</code> was successful. <code>CV_MEM_NULL</code> The CVODE memory block was not initialized through a previous call to <code>CVodeCreate</code> . <code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called. <code>CV_ILL_INPUT</code> 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. (2.6).
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block returned by <code>CVodeCreate</code> . <code>efun</code> ( <code>CVWtFn</code> ) is the C function which defines the <code>ewt</code> vector (see §4.6.3).
Return value	The return value <code>flag</code> (of type <code>int</code> ) will be one of the following: <code>CV_SUCCESS</code> The call to <code>CVodeWftolerances</code> was successful. <code>CV_MEM_NULL</code> The CVODE memory block was not initialized through a previous call to <code>CVodeCreate</code> . <code>CV_NO_MALLOC</code> The allocation function <code>CVodeInit</code> has not been called.

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

(1) The scalar relative tolerance `reltol` is to be set to control relative errors. So `reltol` =  $10^{-4}$  means that errors are controlled to .01%. We do not recommend using `reltol` larger than  $10^{-3}$ .

On the other hand, `reltol` should not be so small that it is comparable to the unit roundoff of the machine arithmetic (generally around 1.0E-15).

(2) The absolute tolerances `abstol` (whether scalar or vector) need to be set to control absolute errors when any components of the solution vector `y` may be so small that pure relative error control is meaningless. For example, if `y[i]` starts at some nonzero value, but in time decays to zero, then pure relative error control on `y[i]` makes no sense (and is overly costly) after `y[i]` is below some noise level. Then `abstol` (if scalar) or `abstol[i]` (if a vector) needs to be set to that noise level. If the different components have different noise levels, then `abstol` should be a vector. See the example `cvRoberts_dns` in the CVODE package, and the discussion of it in the CVODE Examples document [19]. In that problem, the three components vary between 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

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

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

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

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

(3) The user's right-hand side routine `f` should never change a negative value in the solution vector `y` to a non-negative value, as a "solution" to this problem. This can cause instability. If the `f` routine cannot tolerate a zero or negative value (e.g. because there is a square root or log of it), then the offending value should be changed to zero or a tiny positive number in a temporary variable (not in the input `y` vector) for the purposes of computing  $f(t, y)$ .

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

### 4.5.3 Linear solver specification functions

As previously explained, Newton iteration requires the solution of linear systems of the form (2.4). There are eight CVODE linear solvers currently available for this task: `CVDENSE`, `CVBAND`, `CVKLU`, `CVSUPERLUMT`, `CVDIAG`, `CVSPGMR`, `CVSPBCG`, and `CVSPTFQMR`.

The first two linear solvers are direct and derive their names from the type of approximation used for the Jacobian  $J = \partial f / \partial y$ ; `CVDENSE` and `CVBAND` work with dense and banded approximations to  $J$ , respectively. The SUNDIALS suite includes both internal implementations of these two linear solvers and interfaces to Lapack implementations. Together, these linear solvers are referred to as `CVDLS` (from Direct Linear Solvers).

The second two linear solvers are sparse direct solvers based on Gaussian elimination, and require

user-supplied routines to construct the Jacobian  $J = \partial f / \partial y$  in compressed-sparse-column format. The SUNDIALS suite does not include internal implementations of these solver libraries, instead requiring compilation of SUNDIALS to link with existing installations of these libraries (if either is missing, SUNDIALS will install without the corresponding interface routines). Together, these linear solvers are referred to as CVSLs (from Sparse Linear Solvers).

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

The last three CVODE linear solvers, CVSPGMR, CVSPBCG, and CVSPTFQMR, are Krylov iterative solvers, which use scaled preconditioned GMRES, scaled preconditioned Bi-CGStab, and scaled preconditioned TFQMR, respectively. Together, they are referred to as CVSPILS (from Scaled Preconditioned Iterative Linear Solvers).

With any of the Krylov methods, preconditioning can be done on the left only, on the right only, on both the left and the right, or not at all. 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 (2.5).

To specify a CVODE linear solver, after the call to `CVodeCreate` but before any calls to `CVode`, the user's program must call one of the functions `CVDense/CVLapackDense`, `CVBand/CVLapackBand`, `CVKLU`, `CVSuperLUMT`, `CVDiag`, `CVSpgrmr`, `CVSpbcg`, or `CVSptfqmr`, as documented below. The first argument passed to these functions is the CVODE memory pointer returned by `CVodeCreate`. A call to one of these functions links the main CVODE integrator to a linear solver and allows the user to specify parameters which are specific to a particular solver, such as the half-bandwidths in the CVBAND case. The use of each of the 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 linear solver, as specified below.

In each case except the diagonal approximation case CVDIAG, the linear solver module used by CVODE is actually built on top of a generic linear system solver, which may be of interest in itself. These generic solvers, denoted DENSE, BAND, KLU, SUPERLUMT, SPGMR, SPBCG, and SPTFQMR, are described separately in Chapter 8.

#### CVDense

Call `flag = CVDense(cvode_mem, N);`

Description The function `CVDense` selects the CVDENSE linear solver and indicates the use of the internal direct dense linear algebra functions.

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

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

`N` (long int) problem dimension.

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

`CVDL_SUCCESS` The CVDENSE initialization was successful.

`CVDL_MEM_NULL` The `cvode_mem` pointer is `NULL`.

`CVDL_ILL_INPUT` The CVDENSE solver is not compatible with the current NVECTOR module.

`CVDL_MEM_FAIL` A memory allocation request failed.

Notes The CVDENSE linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only `NVECTOR_SERIAL`, `NVECTOR_OPENMP` and `NVECTOR_PTHREADS` are compatible.

#### CVLapackDense

Call `flag = CVLapackDense(cvode_mem, N);`

Description	The function <code>CVLapackDense</code> selects the <code>CVDENSE</code> linear solver and indicates the use of Lapack functions.  The user's main program must include the <code>cvode_lapack.h</code> header file.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVMODE memory block. <code>N</code> ( <code>int</code> ) problem dimension.
Return value	The values of the returned <code>flag</code> (of type <code>int</code> ) are identical to those of <code>CVDense</code> .
Notes	Note that <code>N</code> is restricted to be of type <code>int</code> here, because of the corresponding type restriction in the Lapack solvers.

#### CVBand

Call	<code>flag = CVBand(cvode_mem, N, mupper, mlower);</code>
Description	The function <code>CVBand</code> selects the <code>CVBAND</code> linear solver and indicates the use of the internal direct band linear algebra functions.  The user's main program must include the <code>cvode_band.h</code> header file.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVMODE memory block. <code>N</code> ( <code>long int</code> ) problem dimension. <code>mupper</code> ( <code>long int</code> ) upper half-bandwidth of the problem Jacobian (or of the approximation of it). <code>mlower</code> ( <code>long int</code> ) lower half-bandwidth of the problem Jacobian (or of the approximation of it).
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of:  <code>CVDLS_SUCCESS</code> The <code>CVBAND</code> initialization was successful. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDLS_ILL_INPUT</code> The <code>CVBAND</code> solver is not compatible with the current <code>NVECTOR</code> module, or one of the Jacobian half-bandwidths is outside of its valid range ( $0 \dots N-1$ ). <code>CVDLS_MEM_FAIL</code> A memory allocation request failed.
Notes	The <code>CVBAND</code> linear solver is not compatible with all implementations of the <code>NVECTOR</code> module. Of the <code>NVECTOR</code> modules provided with <code>SUNDIALS</code> , only <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> and <code>NVECTOR_PTHREADS</code> are compatible. The half-bandwidths are to be set such that the nonzero locations $(i, j)$ in the banded (approximate) Jacobian satisfy $-\text{mlower} \leq j - i \leq \text{mupper}$ .

#### CVLapackBand

Call	<code>flag = CVLapackBand(cvode_mem, N, mupper, mlower);</code>
Description	The function <code>CVLapackBand</code> selects the <code>CVBAND</code> linear solver and indicates the use of Lapack functions.  The user's main program must include the <code>cvode_lapack.h</code> header file.
Arguments	The input arguments are identical to those of <code>CVBand</code> , except that <code>N</code> , <code>mupper</code> , and <code>mlower</code> are of type <code>int</code> here.
Return value	The values of the returned <code>flag</code> (of type <code>int</code> ) are identical to those of <code>CVBand</code> .
Notes	Note that <code>N</code> , <code>mupper</code> , and <code>mlower</code> are restricted to be of type <code>int</code> here, because of the corresponding type restriction in the Lapack solvers.

**CVKLU**

Call	<code>flag = CVKLU(cvode_mem, NP, NNZ, sparsetype);</code>
Description	<p>The function <code>CVKLU</code> selects the CVKLU linear solver and indicates the use of sparse-direct linear algebra functions.</p> <p>The user's main program must include the <code>cvode_klu.h</code> header file.</p>
Arguments	<p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block.</p> <p><code>NP</code> (<code>int</code>) problem dimension.</p> <p><code>NNZ</code> (<code>int</code>) maximum number of nonzero entries in the system Jacobian.</p> <p><code>sparsetype</code> (<code>int</code>) sparse storage type of the system Jacobian. If <code>sparsetype</code> is set to <code>CSC_MAT</code> the solver will expect the Jacobian to be stored as a compressed sparse column matrix, and if <code>sparsetype=CSR_MAT</code> the solver will expect a compressed sparse row matrix. If neither option is chosen, the solver will exit with error.</p>
Return value	<p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CVSLS_SUCCESS</code> The CVKLU initialization was successful.</p> <p><code>CVSLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code>.</p> <p><code>CVSLS_ILL_INPUT</code> The CVKLU solver is not compatible with the current NVECTOR module.</p> <p><code>CVSLS_MEM_FAIL</code> A memory allocation request failed.</p> <p><code>CVSLS_PACKAGE_FAIL</code> A call to the KLU library returned a failure flag.</p>
Notes	The CVKLU linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only <code>NVECTOR_SERIAL</code> , <code>NVECTOR_OPENMP</code> and <code>NVECTOR_PTHREADS</code> are compatible.

**CVSuperLUMT**

Call	<code>flag = CVSuperLUMT(cvode_mem, num_threads, N, NNZ);</code>
Description	<p>The function <code>CVSuperLUMT</code> selects the CVSUPERLUMT linear solver and indicates the use of sparse-direct linear algebra functions.</p> <p>The user's main program must include the <code>cvode_superluml.h</code> header file.</p>
Arguments	<p><code>cvode_mem</code> (<code>void *</code>) pointer to the CVODE memory block.</p> <p><code>num_threads</code> (<code>int</code>) the number of threads to use when factoring/solving the linear systems. Note that SuperLU_MT is thread-parallel only in the factorization routine.</p> <p><code>N</code> (<code>int</code>) problem dimension.</p> <p><code>NNZ</code> (<code>int</code>) maximum number of nonzero entries in the system Jacobian.</p>
Return value	<p>The return value <code>flag</code> (of type <code>int</code>) is one of:</p> <p><code>CVSLS_SUCCESS</code> The CVSUPERLUMT initialization was successful.</p> <p><code>CVSLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code>.</p> <p><code>CVSLS_ILL_INPUT</code> The CVSUPERLUMT solver is not compatible with the current NVECTOR module.</p> <p><code>CVSLS_MEM_FAIL</code> A memory allocation request failed.</p> <p><code>CVSLS_PACKAGE_FAIL</code> A call to the SuperLU_MT library returned a failure flag.</p>
Notes	<p>The CVSUPERLUMT linear solver is not compatible with all implementations of the NVECTOR module. Of the NVECTOR modules provided with SUNDIALS, only <code>NVECTOR_SERIAL</code>, <code>NVECTOR_OPENMP</code> and <code>NVECTOR_PTHREADS</code> are compatible.</p> <p>Performance will significantly degrade if the user applies the SuperLU_MT package</p>



compiled with PThreads while using the NVECTOR\_OPENMP module. If a user wants to use a threaded vector kernel with this thread-parallel solver, then SuperLU\_MT should be compiled with openMP and the NVECTOR\_OPENMP module should be used. Also, note that the expected benefit of using the threaded vector kernel is minimal compared to the potential benefit of the threaded solver, unless very long (greater than 100,000 entries) vectors are used.

#### CVDiag

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

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

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

**Return value** The return value `flag` (of type `int`) is one of:  
     CVDIAG\_SUCCESS The CVDIAG initialization was successful.  
     CVDIAG\_MEM\_NULL The `cvode_mem` pointer is NULL.  
     CVDIAG\_ILL\_INPUT The CVDIAG solver is not compatible with the current NVECTOR module.  
     CVDIAG\_MEM\_FAIL A memory allocation request failed.

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

#### CVSpgmr

**Call** `flag = CVSpgmr(cvode_mem, pretype, maxl);`

**Description** The function CVSpgmr selects the CVSPGMR linear solver.  
The user's main program must include the `cvode_spgmr.h` header file.

**Arguments** `cvode_mem` (`void *`) pointer to the CVOICE memory block.  
      (`int`) specifies the preconditioning type and must be one of: `PREC_NONE`, `PREC_LEFT`, `PREC_RIGHT`, or `PREC_BOTH`.  
     maxl (`int`) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value `CVSPILS_MAXL = 5`.

**Return value** The return value `flag` (of type `int`) is one of:  
     CVSPILS\_SUCCESS The CVSPGMR initialization was successful.  
     CVSPILS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
     CVSPILS\_ILL\_INPUT The preconditioner type `pretype` is not valid.  
     CVSPILS\_MEM\_FAIL A memory allocation request failed.

**Notes** The CVSPGMR solver uses a scaled preconditioned GMRES iterative method to solve the linear system (2.4).

#### CVSpgcg

**Call** `flag = CVSpgcg(cvode_mem, pretype, maxl);`

**Description** The function CVSpgcg selects the CVSPBCG linear solver.  
The user's main program must include the `cvode_spgcgs.h` header file.

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

<b>pretype</b>	(int) specifies the preconditioning type and must be one of: <code>PREC_NONE</code> , <code>PREC_LEFT</code> , <code>PREC_RIGHT</code> , or <code>PREC_BOTH</code> .
<b>maxl</b>	(int) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value <code>CVSPILS_MAXL = 5</code> .
Return value	The return value <b>flag</b> (of type <code>int</code> ) is one of <ul style="list-style-type: none"> <li><code>CVSPILS_SUCCESS</code> The CVSPBCG initialization was successful.</li> <li><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</li> <li><code>CVSPILS_ILL_INPUT</code> The preconditioner type <b>pretype</b> is not valid.</li> <li><code>CVSPILS_MEM_FAIL</code> A memory allocation request failed.</li> </ul>
Notes	The CVSPBCG solver uses a scaled preconditioned Bi-CGStab iterative method to solve the linear system (2.4).

#### CVSptfqmr

Call	<code>flag = CVSptfqmr(cvode_mem, pretype, maxl);</code>
Description	The function <code>CVSptfqmr</code> selects the CVSPTFQMR linear solver. The user's main program must include the <code>cvode_sptfqmr.h</code> header file.
Arguments	<b>cvode_mem</b> (void *) pointer to the CVODE memory block. <b>pretype</b> (int) specifies the preconditioning type and must be one of: <code>PREC_NONE</code> , <code>PREC_LEFT</code> , <code>PREC_RIGHT</code> , or <code>PREC_BOTH</code> . <b>maxl</b> (int) maximum dimension of the Krylov subspace to be used. Pass 0 to use the default value <code>CVSPILS_MAXL = 5</code> .
Return value	The return value <b>flag</b> (of type <code>int</code> ) is one of <ul style="list-style-type: none"> <li><code>CVSPILS_SUCCESS</code> The CVSPTFQMR initialization was successful.</li> <li><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.</li> <li><code>CVSPILS_ILL_INPUT</code> The preconditioner type <b>pretype</b> is not valid.</li> <li><code>CVSPILS_MEM_FAIL</code> A memory allocation request failed.</li> </ul>
Notes	The CVSPTFQMR solver uses a scaled preconditioned TFQMR iterative method to solve the linear system (2.4).

#### 4.5.4 Rootfinding initialization function

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

#### CVodeRootInit

Call	<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	<b>cvode_mem</b> (void *) pointer to the CVODE memory block returned by <code>CVodeCreate</code> . <b>nrtfn</b> (int) is the number of root functions $g_i$ . <b>g</b> ( <code>CVRootFn</code> ) is the C function which defines the <b>nrtfn</b> functions $g_i(t, y)$ whose roots are sought. See §4.6.4 for details.
Return value	The return value <b>flag</b> (of type <code>int</code> ) is one of <ul style="list-style-type: none"> <li><code>CV_SUCCESS</code> The call to <code>CVodeRootInit</code> was successful.</li> <li><code>CV_MEM_NULL</code> The <code>cvode_mem</code> argument was NULL.</li> </ul>

	<b>CV_MEM_FAIL</b> A memory allocation failed.
	<b>CV_ILL_INPUT</b> The function <b>g</b> is NULL, but <b>nrtfn</b> > 0.
Notes	If a new IVP is to be solved with a call to <b>CVodeReInit</b> , where the new IVP has no rootfinding problem but the prior one did, then call <b>CVodeRootInit</b> with <b>nrtfn</b> = 0.

#### 4.5.5 CVODE solver function

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

##### CVode

Call	<code>flag = CVode(cvode_mem, tout, yout, &amp;tret, itask);</code>
Description	The function <b>CVode</b> integrates the ODE over an interval in $t$ .
Arguments	<p><b>cvode_mem</b> (void *) pointer to the CVODE memory block.</p> <p><b>tout</b> (realtype) the next time at which a computed solution is desired.</p> <p><b>yout</b> (N_Vector) the computed solution vector.</p> <p><b>tret</b> (realtype) the time reached by the solver (output).</p> <p><b>itask</b> (int) a flag indicating the job of the solver for the next user step. The <b>CV_NORMAL</b> option causes the solver to 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 <math>y(\mathbf{tout})</math>. The <b>CV_ONE_STEP</b> 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><b>CVode</b> returns a vector <b>yout</b> and a corresponding independent variable value <math>t = \mathbf{tret}</math>, such that <b>yout</b> is the computed value of <math>y(t)</math>.</p> <p>In <b>CV_NORMAL</b> mode (with no errors), <b>tret</b> will be equal to <b>tout</b> and <b>yout</b> = <math>y(\mathbf{tout})</math>.</p> <p>The return value <b>flag</b> (of type <b>int</b>) will be one of the following:</p> <p><b>CV_SUCCESS</b> <b>CVode</b> succeeded and no roots were found.</p> <p><b>CV_TSTOP_RETURN</b> <b>CVode</b> succeeded by reaching the stopping point specified through the optional input function <b>CVodeSetStopTime</b> (see §4.5.6.1).</p> <p><b>CV_ROOT_RETURN</b> <b>CVode</b> succeeded and found one or more roots. In this case, <b>tret</b> is the location of the root. If <b>nrtfn</b> &gt; 1, call <b>CVodeGetRootInfo</b> to see which <math>g_i</math> were found to have a root.</p> <p><b>CV_MEM_NULL</b> The <b>cvode_mem</b> argument was NULL.</p> <p><b>CV_NO_MALLOC</b> The CVODE memory was not allocated by a call to <b>CVodeInit</b>.</p> <p><b>CV_ILL_INPUT</b> One of the inputs to <b>CVode</b> 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 <b>CVodeCreate</b>) failed to set the linear solver-specific <b>lsolve</b> field in <b>cvode_mem</b>. (d) A root of one of the root functions was found both at a point <math>t</math> and also very near <math>t</math>. In any case, the user should see the error message for details.</p> <p><b>CV_TOO_CLOSE</b> The initial time <math>t_0</math> and the final time <math>t_{out}</math> are too close to each other and the user did not specify an initial step size.</p> <p><b>CV_TOO_MUCH_WORK</b> The solver took <b>mxstep</b> internal steps but still could not reach <b>tout</b>. The default value for <b>mxstep</b> is <b>MXSTEP_DEFAULT</b> = 500.</p>

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 ( $\text{MXNEF} = 7$ ) during one internal time step, or with $ h  = h_{\min}$ .
CV_CONV_FAILURE	Either convergence test failures occurred too many times ( $\text{MXNCF} = 10$ ) 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.

### 4.5.6 Optional input functions

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

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

#### 4.5.6.1 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.

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

Optional input	Function name	Default
<b>CVODE main solver</b>		
Pointer to an error file	CVodeSetErrFile	stderr
Error handler function	CVodeSetErrHandlerFn	internal fn.
User data	CVodeSetUserData	NULL
Maximum order for BDF method	CVodeSetMaxOrd	5
Maximum order for Adams method	CVodeSetMaxOrd	12
Maximum no. of internal steps before $t_{\text{out}}$	CVodeSetMaxNumSteps	500
Maximum no. of warnings for $t_n + h = t_n$	CVodeSetMaxHnilWarns	10
Flag to activate stability limit detection	CVodeSetStabLimDet	FALSE
Initial step size	CVodeSetInitStep	estimated
Minimum absolute step size	CVodeSetMinStep	0.0
Maximum absolute step size	CVodeSetMaxStep	$\infty$
Value of $t_{\text{stop}}$	CVodeSetStopTime	undefined
Maximum no. of error test failures	CVodeSetMaxErrTestFails	7
Maximum no. of nonlinear iterations	CVodeSetMaxNonlinIters	3
Maximum no. of convergence failures	CVodeSetMaxConvFails	10
Coefficient in the nonlinear convergence test	CVodeSetNonlinConvCoef	0.1
Nonlinear iteration type	CVodeSetIterType	none
Direction of zero-crossing	CVodeSetRootDirection	both
Disable rootfinding warnings	CVodeSetNoInactiveRootWarn	none
<b>CVDLS linear solvers</b>		
Dense Jacobian function	CVDlsSetDenseJacFn	DQ
Band Jacobian function	CVDlsSetBandJacFn	DQ
<b>CVSLS linear solvers</b>		
Sparse Jacobian function	CVSlsSetSparseJacFn	none
Sparse matrix ordering algorithm	CVKLUSetOrdering	1 for COLAMD
Sparse matrix ordering algorithm	CVSuperLUMTSetOrdering	3 for COLAMD
<b>CVSPILS linear solvers</b>		
Preconditioner functions	CVSpilsSetPreconditioner	NULL, NULL
Jacobian-times-vector function	CVSpilsSetJacTimesVecFn	DQ
Preconditioning type	CVSpilsSetPrecType	none
Ratio between linear and nonlinear tolerances	CVSpilsSetEpsLin	0.05
Type of Gram-Schmidt orthogonalization <sup>(a)</sup>	CVSpilsSetGSType	modified GS
Maximum Krylov subspace size <sup>(b)</sup>	CVSpilsSetMaxl	5

<sup>(a)</sup> Only for CVSPGMR<sup>(b)</sup> Only for CVSPBCG and CVSPTFQMR

**CVodeSetErrFile**

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

**CVodeSetErrHandlerFn**

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

**CVodeSetUserData**

Call	<code>flag = CVodeSetUserData(cvode_mem, user_data);</code>
Description	The function <code>CVodeSetUserData</code> specifies the user data block <code>user_data</code> and attaches it to the main CVODE memory block.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>user_data</code> (void *) pointer to the user data.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	If specified, the pointer to <code>user_data</code> is passed to all user-supplied functions that have it as an argument. Otherwise, a NULL pointer is passed.  If <code>user_data</code> is needed in user linear solver or preconditioner functions, the call to <code>CVodeSetUserData</code> must be made <i>before</i> the call to specify the linear solver.



**CVodeSetMaxOrd**

Call	<code>flag = CVodeSetMaxOrder(cvode_mem, maxord);</code>
Description	The function <code>CVodeSetMaxOrder</code> specifies the maximum order of the linear multistep method.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>maxord</code> (int) value of the maximum method order. This must be positive.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CV_ILL_INPUT</code> The specified value <code>maxord</code> is $\leq 0$ , or larger than its previous value.
Notes	The default value is <code>ADAMS_Q_MAX = 12</code> for the Adams-Moulton method and <code>BDF_Q_MAX = 5</code> for the BDF method. Since <code>maxord</code> affects the memory requirements for the internal CVODE memory block, its value cannot be increased past its previous value. An input value greater than the default will result in the default value.

**CVodeSetMaxNumSteps**

Call	<code>flag = CVodeSetMaxNumSteps(cvode_mem, mxsteps);</code>
Description	The function <code>CVodeSetMaxNumSteps</code> specifies the maximum number of steps to be taken by the solver in its attempt to reach the next output time.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>mxsteps</code> (long int) maximum allowed number of steps.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .
Notes	Passing <code>mxsteps = 0</code> results in CVODE using the default value (500). Passing <code>mxsteps &lt; 0</code> disables the test ( <i>not recommended</i> ).

**CVodeSetMaxHnilWarns**

Call	<code>flag = CVodeSetMaxHnilWarns(cvode_mem, mxhnil);</code>
Description	The function <code>CVodeSetMaxHnilWarns</code> specifies the maximum number of messages issued by the solver warning that $t + h = t$ on the next internal step.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>mxhnil</code> (int) maximum number of warning messages ( $> 0$ ).
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> .
Notes	The default value is 10. A negative value for <code>mxhnil</code> indicates that no warning messages should be issued.

**CVodeSetStabLimDet**

Call	<code>flag = CVodeSetstabLimDet(cvode_mem, stldet);</code>
Description	The function <code>CVodeSetStabLimDet</code> indicates if the BDF stability limit detection algorithm should be used. See §2.3 for further details.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block.

**stldet** (booleantype) flag controlling stability limit detection (TRUE = on; FALSE = 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 **FALSE**. If **stldet** = **TRUE** 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 CVODE memory block.

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

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

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

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

Notes By default, CVODE estimates the initial step size to be the solution  $h$  of the equation  $\|0.5h^2\ddot{y}\|_{\text{WRMS}} = 1$ , where  $\ddot{y}$  is an estimated second derivative of the solution at  $t_0$ .

#### CVodeSetMinStep

Call **flag** = **CVodeSetMinStep**(**cvode\_mem**, **hmin**);

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

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

**hmin** (realtype) minimum absolute value of the step size ( $\geq 0.0$ ).

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

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

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

**CV\_ILL\_INPUT** Either **hmin** is nonpositive or it exceeds the maximum allowable step size.

Notes The default value is 0.0.

#### CVodeSetMaxStep

Call **flag** = **CVodeSetMaxStep**(**cvode\_mem**, **hmax**);

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

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

**hmax** (realtype) maximum absolute value of the step size ( $\geq 0.0$ ).

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

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

**CV\_MEM\_NULL** The **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 CVODE memory block. <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 <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <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 CVODE memory block. <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 <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	The default value 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 CVODE memory block. <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 <code>CV_SUCCESS</code> The optional value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	The default value 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 CVODE memory block. <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 <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 CVODE memory block.  
`nlscoef` (realtype) coefficient in nonlinear convergence test ( $> 0.0$ ).

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

Notes The default value is 0.1.

#### 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 CVODE 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 Dense/band direct linear solvers optional input functions

The CVDENSE solver needs a function to compute a dense approximation to the Jacobian matrix  $J(t, y)$ . This function must be of type `CVDlsDenseJacFn`. The user can supply his/her own dense Jacobian function, or use the default internal difference quotient approximation that comes with the CVDENSE solver. To specify a user-supplied Jacobian function `djac`, CVDENSE provides the function `CVDlsSetDenseJacFn`. The CVDENSE solver passes the pointer `user_data` to the dense 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`.

#### CVDlsSetDenseJacFn

Call `flag = CVDlsSetDenseJacFn(cvode_mem, djac);`

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

Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
`djac` (`CVDlsDenseJacFn`) user-defined dense Jacobian approximation function.

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

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

Notes By default, CVDENSE uses an internal difference quotient function. If NULL is passed to `djac`, this default function is used.

The function type `CVDlsDenseJacFn` is described in §4.6.5.

The CVBAND solver needs a function to compute a banded approximation to the Jacobian matrix  $J(t, y)$ . This function must be of type `CVDlsBandJacFn`. The user can supply his/her own banded Jacobian approximation function, or use the default internal difference quotient approximation that comes with the CVBAND solver. To specify a user-supplied Jacobian function `bjac`, CVBAND provides the function `CVDlsSetBandJacFn`. The CVBAND solver passes the pointer `user_data` to the banded Jacobian approximation 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`.

#### `CVDlsSetBandJacFn`

Call `flag = CVDlsSetBandJacFn(cvode_mem, bjac);`  
 Description The function `CVDlsSetBandJacFn` specifies the banded Jacobian approximation function to be used.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           **bjac** (CVBandJacFn) user-defined banded Jacobian approximation function.  
 Return value The return value `flag` (of type `int`) is one of  
           CVDLS\_SUCCESS The optional value has been successfully set.  
           CVDLS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
           CVDLS\_LMEM\_NULL The CVBAND linear solver has not been initialized.  
 Notes By default, CVBAND uses an internal difference quotient function. If NULL is passed to `bjac`, this default function is used.  
 The function type `CVBandJacFn` is described in §4.6.6.

#### 4.5.6.3 Sparse direct linear solvers optional input functions

The CVKLU and CVSUPERLUMT solvers require a function to compute a compressed-sparse-column approximation to the Jacobian matrix  $J(t, y)$ . This function must be of type `CVSlsSparseJacFn`. The user must supply a custom sparse Jacobian function since a difference-quotient approximation would not leverage the underlying sparse matrix structure of the problem. To specify a user-supplied Jacobian function `sjac`, CVKLU and CVSUPERLUMT provide the function `CVSlsSetSparseJacFn`. The CVKLU and CVSUPERLUMT solvers pass the pointer `user_data` to the sparse Jacobian function. This mechanism 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`.

#### `CVSlsSetSparseJacFn`

Call `flag = CVSlsSetSparseJacFn(cvode_mem, sjac);`  
 Description The function `CVSlsSetSparseJacFn` specifies the sparse Jacobian approximation function to be used.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           **sjac** (CVSlsSparseJacFn) user-defined sparse Jacobian approximation function.  
 Return value The return value `flag` (of type `int`) is one of

CVSLS\_SUCCESS The sparse Jacobian routine pointer has been successfully set.  
 CVSLS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
 CVSLS\_LMEM\_NULL The CVKLU or CVSUPERLUMT linear solver has not been initialized.

Notes The function type `CVSlsSparseJacFn` is described in §4.6.7.

When using a sparse direct solver, there may be instances when the number of state variables does not change, but the number of nonzeros in the Jacobian does change. In this case, for the CVKLU solver, we provide the following reinitialization function. This function reinitializes the Jacobian matrix memory for the new number of nonzeros and sets 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 where the structure of the linear system has changed, requiring a new symbolic (and numeric) factorization.

#### CVKLUREInit

Call `flag = CVKLUREInit(cv_mem, n, nnz, reinit_type);`

Description The function `CVKLUREInit` reinitializes Jacobian matrix memory and flags for new symbolic and numeric KLU factorizations.

Arguments `cv_mem` (`void *`) pointer to the CVODE memory block.  
`n` (`int`) number of state variables in the system.  
`nnz` (`int`) number of nonzeros in the Jacobian matrix.  
`reinit_type` (`int`) type of reinitialization:

- 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 prior call to CVKLU.

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

CVSLS\_SUCCESS The reinitialization succeeded.  
 CVSLS\_MEM\_NULL The `cv_mem` pointer is NULL.  
 CVSLS\_LMEM\_NULL The CVKLU linear solver has not been initialized.  
 CVSLS\_ILL\_INPUT The given `reinit_type` has an illegal value.  
 CVSLS\_MEM\_FAIL A memory allocation failed.

Notes The default value for `reinit_type` is 2.

Both the CVKLU and CVSUPERLUMT solvers can apply reordering algorithms to minimize fill-in for the resulting sparse *LU* decomposition internal to the solver. The approximate minimal degree ordering for nonsymmetric matrices given by the COLAMD algorithm is the default algorithm used within both solvers, but alternate orderings may be chosen through one of the following two functions. The input values to these functions are the numeric values used in the respective packages, and the user-supplied value will be passed directly to the package.

#### CVKLUSetOrdering

Call `flag = CVKLUSetOrdering(cv_mem, ordering_choice);`

Description The function `CVKLUSetOrdering` specifies the ordering algorithm used by CVKLU for reducing fill.

Arguments `cv_mem` (`void *`) pointer to the CVODE memory block.  
`ordering_choice` (`int`) flag denoting algorithm choice:

0 AMD

- 1 COLAMD
- 2 natural ordering

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

- CVSLS\_SUCCESS The optional value has been successfully set.
- CVSLS\_MEM\_NULL The `cv_mem` pointer is NULL.
- CVSLS\_ILL\_INPUT The supplied value of `ordering_choice` is illegal.

Notes The default ordering choice is 1 for COLAMD.

#### CVSuperLUMTSetOrdering

Call `flag = CVSuperLUMTSetOrdering(cv_mem, ordering_choice);`

Description The function `CVSuperLUMTSetOrdering` specifies the ordering algorithm used by CVSUPERLUMT for reducing fill.

Arguments `cv_mem` (`void *`) pointer to the CVODE memory block.  
`ordering_choice` (`int`) flag denoting algorithm choice:

- 0 natural ordering
- 1 minimal degree ordering on  $J^T J$
- 2 minimal degree ordering on  $J^T + J$
- 3 COLAMD

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

- CVSLS\_SUCCESS The optional value has been successfully set.
- CVSLS\_MEM\_NULL The `cv_mem` pointer is NULL.
- CVSLS\_ILL\_INPUT The supplied value of `ordering_choice` is illegal.

Notes The default ordering choice is 3 for COLAMD.

#### 4.5.6.4 Iterative linear solvers optional input functions

If any preconditioning is to be done within one of the CVSPILS linear solvers, 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.

Ther CVSPILS solvers require a function to compute an approximation to the product between the Jacobian matrix  $J(t, y)$  and a vector  $v$ . The user can supply his/her own Jacobian-times-vector approximation function, or use the default internal difference quotient function that comes with the CVSPILS solvers. A user-defined Jacobian-vector function must be of type `CVSpilsJacTimesVecFn` and can be specified through a call to `CVSpilsSetJacTimesVecFn` (see §4.6.8 for specification details). As with the preconditioner user-supplied 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 function `jt看` each time it is called.

**CVSpilsSetPreconditioner**

Call	<code>flag = CVSpilsSetPreconditioner(cvode_mem, psetup, psolve);</code>
Description	The function <code>CVSpilsSetPreconditioner</code> specifies the preconditioner setup and solve functions.
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>psetup</code> (<code>CVSpilsPrecSetupFn</code>) user-defined preconditioner setup function. Pass NULL if no setup is to be done.</p> <p><code>psolve</code> (<code>CVSpilsPrecSolveFn</code>) user-defined preconditioner solve 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 values have 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>
Notes	The function type <code>CVSpilsPrecSolveFn</code> is described in §4.6.9. The function type <code>CVSpilsPrecSetupFn</code> is described in §4.6.10.

**CVSpilsSetJacTimesVecFn**

Call	<code>flag = CVSpilsSetJacTimesVecFn(cvode_mem, jtimes);</code>
Description	The function <code>CVSpilsSetJacTimesFn</code> specifies the Jacobian-vector function to be used.
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>jtimes</code> (<code>CVSpilsJacTimesVecFn</code>) 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>
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>CVSpilsJacTimesVecFn</code> is described in §4.6.8.</p>

**CVSpilsSetPrecType**

Call	<code>flag = CVSpilsSetPrecType(cvode_mem, pretype);</code>
Description	The function <code>CVSpilsSetPrecType</code> resets the type of preconditioning to be used.
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>pretype</code> (int) specifies the type of preconditioning and must be one of: <code>PREC_NONE</code>, <code>PREC_LEFT</code>, <code>PREC_RIGHT</code>, or <code>PREC_BOTH</code>.</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 preconditioner type <code>pretype</code> is not valid.</p>
Notes	The preconditioning type is initially set in the call to the linear solver's specification function (see §4.5.3). This function call is needed only if <code>pretype</code> is being changed from its original value.

**CVSpilsSetGSType**

Call	<code>flag = CVSpilsSetGSType(cvode_mem, gstype);</code>
Description	The function <code>CVSpilsSetGSType</code> specifies the Gram-Schmidt orthogonalization to be used with the CVSPGMR solver (one of the enumeration constants <code>MODIFIED_GS</code> or <code>CLASSICAL_GS</code> ). These correspond to using modified Gram-Schmidt and classical Gram-Schmidt, respectively.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block. <code>gstype</code> (int) type of Gram-Schmidt orthogonalization.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized. <code>CVSPILS_ILL_INPUT</code> The value of <code>gstype</code> is not valid.
Notes	The default value is <code>MODIFIED_GS</code> . This option is available only for the CVSPGMR linear solver.

**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	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block. <code>eplifac</code> (realtype) linear convergence safety factor ( $\geq 0.0$ ).
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized. <code>CVSPILS_ILL_INPUT</code> The factor <code>eplifac</code> is negative.
Notes	The default value is 0.05. Passing a value <code>eplifac</code> = 0.0 also indicates using the default value.

**CVSpilsSetMaxl**

Call	<code>flag = CVSpilsSetMaxl(cv_mem, maxl);</code>
Description	The function <code>CVSpilsSetMaxl</code> resets the maximum Krylov subspace dimension for the Bi-CGSTab or TFQMR methods.
Arguments	<code>cv_mem</code> (void *) pointer to the CVOICE memory block. <code>maxl</code> (int) maximum dimension of the Krylov subspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized. <code>CVSPILS_ILL_INPUT</code> The current linear solver is SPGMR.
Notes	The maximum subspace dimension is initially specified in the call to the linear solver specification function (see §4.5.3). This function call is needed only if <code>maxl</code> is being changed from its previous value. An input value <code>maxl</code> $\leq 0$ will result in the default value, 5. This option is available only for the CVSPBCG and CVSPTFQMR linear solvers.



#### 4.5.6.5 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 CVODE 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	<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_ILL_INPUT</code> rootfinding has not been activated through a call to <code>CVodeRootInit</code>.</p>
Notes	The default behavior is to monitor for both zero-crossing directions.

##### **CVodeSetNoInactiveRootWarn**

Call	<code>flag = CVodeSetNoInactiveRootWarn(cvode_mem);</code>
Description	The function <code>CVodeSetNoInactiveRootWarn</code> disables issuing a warning if some root function appears to be identically zero at the beginning of the integration.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block.
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>
Notes	CVODE will not report the initial conditions as a possible zero-crossing (assuming that one or more components $g_i$ are zero at the initial time). However, if it appears that some $g_i$ is identically zero at the initial time (i.e., $g_i$ is zero at the initial time and after the first step), CVODE will issue a warning which can be disabled with this optional input function.

#### 4.5.7 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 CVODE.

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

##### **CVodeGetDky**

Call	<code>flag = CVodeGetDky(cvode_mem, t, k, dky);</code>
Description	<p>The function <code>CVodeGetDky</code> computes the <math>k</math>-th derivative of the function <math>y</math> at time <math>t</math>, i.e. <math>d^{(k)}y/dt^{(k)}(t)</math>, where <math>t_n - h_u \leq t \leq t_n</math>, <math>t_n</math> denotes the current internal time reached, and <math>h_u</math> is the last internal step size successfully used by the solver. The user may request <math>k = 0, 1, \dots, q_u</math>, where <math>q_u</math> is the current order (optional output <code>qlast</code>).</p>

Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>t</code> (realtype) the value of the independent variable at which the derivative is to be evaluated.</p> <p><code>k</code> (int) the derivative order requested.</p> <p><code>dky</code> (N_Vector) vector containing the derivative. This vector must be allocated by the user.</p>
Return value	<p>The return value <code>flag</code> (of type <code>int</code>) is one of</p> <p><code>CV_SUCCESS</code> <code>CVodeGetDky</code> succeeded.</p> <p><code>CV_BAD_K</code> <code>k</code> is not in the range <math>0, 1, \dots, q_u</math>.</p> <p><code>CV_BAD_T</code> <code>t</code> is not in the interval <math>[t_n - h_u, t_n]</math>.</p> <p><code>CV_BAD_DKY</code> The <code>dky</code> argument was <code>NULL</code>.</p> <p><code>CV_MEM_NULL</code> The <code>cvode_mem</code> argument was <code>NULL</code>.</p>
Notes	<p>It is only legal to call the function <code>CVodeGetDky</code> after a successful return from <code>CVode</code>. See <code>CVodeGetCurrentTime</code>, <code>CVodeGetLastOrder</code>, and <code>CVodeGetLastStep</code> in the next section for access to <math>t_n</math>, <math>q_u</math>, and <math>h_u</math>, respectively.</p>

### 4.5.8 Optional output functions

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

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

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

##### CVodeGetWorkSpace

Call	<code>flag = CVodeGetWorkSpace(cvode_mem, &amp;lenrw, &amp;leniw);</code>
Description	The function <code>CVodeGetWorkSpace</code> returns the CVODE real and integer workspace sizes.
Arguments	<p><code>cvode_mem</code> (void *) pointer to the CVODE memory block.</p> <p><code>lenrw</code> (long int) the number of <code>realtype</code> values in the CVODE workspace.</p> <p><code>leniw</code> (long int) the number of integer values in the CVODE workspace.</p>

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

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

- 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: `lenrw = 96 + (maxord+5) *  $N_r$  + 3*nrtfn`;
  - using `CVodeSVtolerances`: `lenrw = lenrw +  $N_r$` ;
- where  $N_r$  is the number of real words in one `N_Vector` ( $\approx N$ ).
- The size of the integer workspace (without distinction between `int` and `long int` words) is given by:
- base value: `leniw = 40 + (maxord+5) *  $N_i$  + nrtfn`;
  - using `CVodeSVtolerances`: `leniw = leniw +  $N_i$` ;
- where  $N_i$  is the number of integer words in one `N_Vector` ( $= 1$  for `NVECTOR_SERIAL` and  $2*\texttt{npes}$  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: `lenrw = 96 + 17 $N$`  and `leniw = 57`
  - For the BDF method: `lenrw = 96 + 10 $N$`  and `leniw = 50`

#### CVodeGetNumSteps

- Call** `flag = CVodeGetNumSteps(cvode_mem, &nsteps);`
- Description** The function `CVodeGetNumSteps` returns the cumulative number of internal steps taken by the solver (total so far).
- Arguments** `cvode_mem` (`void *`) pointer to the CVODE memory block.  
`nsteps` (`long int`) number of steps taken by CVODE.
- Return value** The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
  - `CV_MEM_NULL` The `cvode_mem` pointer is `NULL`.

#### CVodeGetNumRhsEvals

- Call** `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 CVODE memory block.  
`nfevals` (`long int`) number of calls to the user's `f` function.
- Return value** The return value `flag` (of type `int`) is one of
- `CV_SUCCESS` The optional output value has been successfully set.
  - `CV_MEM_NULL` The `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 CVODE memory block.  
                  `nlinsetups` (long int) number of calls made to the linear solver setup function.

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

`CV_SUCCESS`   The optional output value has been successfully set.  
                  `CV_MEM_NULL`   The `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 CVODE memory block.  
                  `netfails`   (long int) number of error test failures.

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

`CV_SUCCESS`   The optional output value has been successfully set.  
                  `CV_MEM_NULL`   The `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 CVODE memory block.  
                  `qlast`        (int) method order used on the last internal step.

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

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

**CVodeGetCurrentOrder**

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

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

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

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

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

**CVodeGetLastStep**

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

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

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

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

**CVodeGetCurrentStep**

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

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

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

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

**CVodeGetActualInitStep**

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

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

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

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

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

**CVodeGetCurrentTime**

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

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

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

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

**CVodeGetNumStabLimOrderReds**

Call	<code>flag = CVodeGetNumStabLimOrderReds(cvode_mem, &amp;nsired);</code>
Description	The function <code>CVodeGetNumStabLimOrderReds</code> returns the number of order reductions dictated by the BDF stability limit detection algorithm (see §2.3).
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nsired</code> (long int) number of order reductions due to stability limit detection.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	If the stability limit detection algorithm was not initialized ( <code>CVodeSetStabLimDet</code> was not called), then <code>nsired = 0</code> .

**CVodeGetTolScaleFactor**

Call	<code>flag = CVodeGetTolScaleFactor(cvode_mem, &amp;tolsfac);</code>
Description	The function <code>CVodeGetTolScaleFactor</code> 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	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>tolsfac</code> (realtype) suggested scaling factor for user-supplied tolerances.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.

**CVodeGetErrWeights**

Call	<code>flag = CVodeGetErrWeights(cvode_mem, eweight);</code>
Description	The function <code>CVodeGetErrWeights</code> returns the solution error weights at the current time. These are the reciprocals of the $W_i$ given by (2.6).
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>eweight</code> (N_Vector) solution error weights at the current time.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.
Notes	The user must allocate memory for <code>eweight</code> .

**CVodeGetEstLocalErrors**

Call	<code>flag = CVodeGetEstLocalErrors(cvode_mem, ele);</code>
Description	The function <code>CVodeGetEstLocalErrors</code> returns the vector of estimated local errors.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE 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>cvode_mem</code> pointer is NULL.



Notes The user must allocate memory for `ele`.

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

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

#### CVodeGetIntegratorStats

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

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

Arguments

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

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

<code>CV_SUCCESS</code>	the optional output values have been successfully set.
<code>CV_MEM_NULL</code>	the <code>cvode_mem</code> pointer is NULL.

#### CVodeGetNumNonlinSolvIters

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

Description The function `CVodeGetNumNonlinSolvIters` returns the number of nonlinear (functional or Newton) iterations performed.

Arguments

<code>cvode_mem</code>	(void *) pointer to the CVODE memory block.
<code>nniters</code>	(long int) number of nonlinear iterations performed.

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

<code>CV_SUCCESS</code>	The optional output values have been successfully set.
<code>CV_MEM_NULL</code>	The <code>cvode_mem</code> pointer is NULL.

#### CVodeGetNumNonlinSolvConvFails

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

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

Arguments

<code>cvode_mem</code>	(void *) pointer to the CVODE memory block.
------------------------	---

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

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

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

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

#### CVodeGetNonlinSolvStats

Call **flag = CVodeGetNonlinSolvStats(cvode\_mem, &nniters, &nncfails);**

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

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

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

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

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

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

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

#### CVodeGetReturnFlagName

Call **name = CVodeGetReturnFlagName(flag);**

Description The function **CVodeGetReturnFlagName** returns the name of the CVODE constant corresponding to **flag**.

Arguments The only argument, of type **int**, is a return flag from a CVODE function.

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

### 4.5.8.2 Rootfinding optional output functions

There are two optional output functions associated with rootfinding.

#### CVodeGetRootInfo

Call **flag = CVodeGetRootInfo(cvode\_mem, rootsfound);**

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

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

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

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

**CV\_SUCCESS** The optional output values have been successfully set.

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

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

The user must allocate memory for the vector **rootsfound**.



**CVodeGetNumGEvals**

Call	<code>flag = CVodeGetNumGEvals(cvode_mem, &amp;ngevals);</code>
Description	The function <code>CVodeGetNumGEvals</code> returns the cumulative number of calls made to the user-supplied root function <i>g</i> .
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>ngevals</code> (long int) number of calls made to the user's function <i>g</i> thus far.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of: <code>CV_SUCCESS</code> The optional output value has been successfully set. <code>CV_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL.

**4.5.8.3 Dense/band direct linear solvers 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 here (e.g. `lenrwLS`).

**CVDlsGetWorkSpace**

Call	<code>flag = CVDlsGetWorkSpace(cvode_mem, &amp;lenrwLS, &amp;leniwLS);</code>
Description	The function <code>CVDlsGetWorkSpace</code> returns the sizes of the real and integer workspaces used by a CVDLS linear solver (CVDENSE or CVBAND).
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>lenrwLS</code> (long int) the number of <code>realtype</code> values in the CVDLS workspace. <code>leniwLS</code> (long int) the number of integer values in the CVDLS workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDLS_SUCCESS</code> The optional output values have been successfully set. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVDLS_LMEM_NULL</code> The CVDLS linear solver has not been initialized.
Notes	For the CVDENSE linear solver, in terms of the problem size <i>N</i> , the actual size of the real workspace is $2N^2$ <code>realtype</code> words, and the actual size of the integer workspace is <i>N</i> integer words. For the CVBAND linear solver, in terms of <i>N</i> and Jacobian half-bandwidths, the actual size of the real workspace is $(2 \text{ mupper} + 3 \text{ mlower} + 2) N$ <code>realtype</code> words, and the actual size of the integer workspace is <i>N</i> integer words.

**CVDlsGetNumJacEvals**

Call	<code>flag = CVDlsGetNumJacEvals(cvode_mem, &amp;njevals);</code>
Description	The function <code>CVDlsGetNumJacEvals</code> returns the number of calls made to the CVDLS (dense or band) Jacobian approximation function.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>njevals</code> (long int) the number of calls to the Jacobian function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDLS_SUCCESS</code> The optional output value has been successfully set. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVDLS_LMEM_NULL</code> The CVDLS linear solver has not been initialized.

**CVDlsGetNumRhsEvals**

Call	<code>flag = CVDlsGetNumRhsEvals(cvode_mem, &amp;nfevalsLS);</code>
Description	The function <code>CVDlsGetNumRhsEvals</code> returns the number of calls made to the user-supplied right-hand side function due to the finite difference (dense or band) Jacobian approximation.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>nfevalsLS</code> ( <code>long int</code> ) the number of calls made to the user-supplied right-hand side function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDLS_SUCCESS</code> The optional output value has been successfully set. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDLS_LMEM_NULL</code> The CVDLS linear solver has not been initialized.
Notes	The value <code>nfevalsLS</code> is incremented only if the default internal difference quotient function is used.

**CVDlsGetLastFlag**

Call	<code>flag = CVDlsGetLastFlag(cvode_mem, &amp;lsflag);</code>
Description	The function <code>CVDlsGetLastFlag</code> returns the last return value from a CVDLS routine.
Arguments	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVODE memory block. <code>lsflag</code> ( <code>long int</code> ) the value of the last return flag from a CVDLS function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVDLS_SUCCESS</code> The optional output value has been successfully set. <code>CVDLS_MEM_NULL</code> The <code>cvode_mem</code> pointer is <code>NULL</code> . <code>CVDLS_LMEM_NULL</code> The CVDLS linear solver has not been initialized.
Notes	If the <code>CVDENSE</code> setup function failed ( <code>CVode</code> returned <code>CV_LSETUP_FAIL</code> ), then the value of <code>lsflag</code> 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. For all other failures, <code>lsflag</code> is negative.

**CVDlsGetReturnFlagName**

Call	<code>name = CVDlsGetReturnFlagName(lsflag);</code>
Description	The function <code>CVDlsGetReturnFlagName</code> returns the name of the CVDLS constant corresponding to <code>lsflag</code> .
Arguments	The only argument, of type <code>long int</code> , 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”.

**4.5.8.4 Diagonal linear solver 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 CVOICE 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 CVOICE 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 CVOICE 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            `name = CVDiagGetReturnFlagName(lsflag);`

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

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

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

**4.5.8.5 Sparse direct linear solvers optional output functions**

The following optional outputs are available from the CVSLS modules: number of calls to the Jacobian routine and last return value from a CVSLS function.

**CVSlsGetNumJacEvals**

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

Description    The function `CVSlsGetNumJacEvals` returns the number of calls made to the CVSLS sparse Jacobian approximation function.

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

`njevals`    (`long int`) the number of calls to the Jacobian function.

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

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

`CVSLS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.

`CVSLS_LMEM_NULL`    The CVSLS linear solver has not been initialized.

**CVSlsGetLastFlag**

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

Description    The function `CVSlsGetLastFlag` returns the last return value from a CVSLS routine.

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

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

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

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

`CVSLS_MEM_NULL`    The `cvode_mem` pointer is `NULL`.

`CVSLS_LMEM_NULL`    The CVSLS linear solver has not been initialized.

Notes

**CVSlsGetReturnFlagName**

Call            `name = CVSlsGetReturnFlagName(lsflag);`

Description    The function `CVSlsGetReturnFlagName` returns the name of the CVSLS constant corresponding to `lsflag`.

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

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

#### 4.5.8.6 Iterative linear solvers 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 product routine, 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 here (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 CVODE memory block. <code>lenrwLS</code> (long int) the number of <code>realtype</code> values in the CVSPILS workspace. <code>leniwLS</code> (long int) the number of integer values in the CVSPILS workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.
Notes	In terms of the problem size $N$ and maximum subspace size <code>maxl</code> , the actual size of the real workspace is roughly: $(\text{maxl}+5) * N + \text{maxl} * (\text{maxl}+4) + 1$ <code>realtype</code> words for CVSPGMR, $9 * N$ <code>realtype</code> words for CVSPBCG, and $11 * N$ <code>realtype</code> words for CVSPTFQMR. In a parallel setting, the above values are global, 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 CVODE memory block. <code>nliters</code> (long int) the current number of linear iterations.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer is NULL. <code>CVSPILS_LMEM_NULL</code> The CVSPILS linear solver has not been initialized.

##### CVSpilsGetNumConvFails

Call	<code>flag = CVSpilsGetNumConvFails(cvode_mem, &amp;nlcfails);</code>
Description	The function <code>CVSpilsGetNumConvFails</code> returns the cumulative number of linear convergence failures.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nlcfails</code> (long int) the current number of linear convergence failures.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of

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.

#### 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 = FALSE`.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `npevals` (long int) the current number of calls to `psetup`.  
 Return value The return value `flag` (of type `int`) is one of  
           CVSPILS\_SUCCESS The optional output value has been successfully set.  
           CVSPILS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
           CVSPILS\_LMEM\_NULL The CVSPILS linear solver has not been initialized.

#### CVSpilsGetNumPrecSolves

Call `flag = CVSpilsGetNumPrecSolves(cvode_mem, &npsolves);`  
 Description The function `CVSpilsGetNumPrecSolves` returns the cumulative number of calls made to the preconditioner solve function, `psolve`.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `npsolves` (long int) the current number of calls to `psolve`.  
 Return value The return value `flag` (of type `int`) is one of  
           CVSPILS\_SUCCESS The optional output value has been successfully set.  
           CVSPILS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
           CVSPILS\_LMEM\_NULL The CVSPILS linear solver has not been initialized.

#### CVSpilsGetNumJtimesEvals

Call `flag = CVSpilsGetNumJtimesEvals(cvode_mem, &njvevals);`  
 Description The function `CVSpilsGetNumJtimesEvals` returns the cumulative number made to the Jacobian-vector function, `jtimes`.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `njvevals` (long int) the current number of calls to `jtimes`.  
 Return value The return value `flag` (of type `int`) is one of  
           CVSPILS\_SUCCESS The optional output value has been successfully set.  
           CVSPILS\_MEM\_NULL The `cvode_mem` pointer is NULL.  
           CVSPILS\_LMEM\_NULL The CVSPILS linear solver has not been initialized.

#### CVSpilsGetNumRhsEvals

Call `flag = CVSpilsGetNumRhsEvals(cvode_mem, &nfevalsLS);`  
 Description The function `CVSpilsGetNumRhsEvals` returns the number of calls to the user right-hand side function for finite difference Jacobian-vector product approximation.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `nfevalsLS` (long int) the number of calls to the user right-hand side function.  
 Return value The return value `flag` (of type `int`) is one of

	<code>CVSPILS_SUCCESS</code>	The optional output value has been successfully set.
	<code>CVSPILS_MEM_NULL</code>	The <code>cvode_mem</code> pointer is NULL.
	<code>CVSPILS_LMEM_NULL</code>	The CVSPILS linear solver has not been initialized.
Notes	The value <code>nfevalsLS</code> is incremented only if the default <code>CVSpilsDQJtimes</code> difference quotient function is used.	

#### CVSpilsGetLastFlag

Call	<code>flag = CVSpilsGetLastFlag(cvode_mem, &amp;lsflag);</code>	
Description	The function <code>CVSpilsGetLastFlag</code> returns the last return value from a CVSPILS routine.	
Arguments	<code>cvode_mem</code> (void *) pointer to the CVOICE memory block.	
	<code>lsflag</code> (long int) the value of the last return flag from a CVSPILS function.	
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of	
	<code>CVSPILS_SUCCESS</code>	The optional output value has been successfully set.
	<code>CVSPILS_MEM_NULL</code>	The <code>cvode_mem</code> pointer is NULL.
	<code>CVSPILS_LMEM_NULL</code>	The CVSPILS linear solver has not been initialized.
Notes	<p>If the CVSPILS setup function failed (CVOICE returned <code>CV_LSETUP_FAIL</code>), <code>lsflag</code> will be <code>SPGMR_PSET_FAIL_UNREC</code>, <code>SPBCG_PSET_FAIL_UNREC</code>, or <code>SPTFQMR_PSET_FAIL_UNREC</code>.</p> <p>If the CVSPGMR solve function failed (CVOICE returned <code>CV_LSOLVE_FAIL</code>), <code>lsflag</code> contains the error return flag from <code>SpgmrSolve</code> and will be one of: <code>SPGMR_MEM_NULL</code>, indicating that the SPGMR memory is NULL; <code>SPGMR_ATIMES_FAIL_UNREC</code>, indicating an unrecoverable failure in the <math>J*v</math> function; <code>SPGMR_PSOLVE_FAIL_UNREC</code>, indicating that the preconditioner solve function <code>psolve</code> failed unrecoverably; <code>SPGMR_GS_FAIL</code>, indicating a failure in the Gram-Schmidt procedure; or <code>SPGMR_QRSOL_FAIL</code>, indicating that the matrix <math>R</math> was found to be singular during the QR solve phase.</p> <p>If the CVSPBCG solve function failed (CVOICE returned <code>CV_LSOLVE_FAIL</code>), <code>lsflag</code> contains the error return flag from <code>SpbcgSolve</code> and will be one of: <code>SPBCG_MEM_NULL</code>, indicating that the SPBCG memory is NULL; <code>SPBCG_ATIMES_FAIL_UNREC</code>, indicating an unrecoverable failure in the <math>J*v</math> function; or <code>SPBCG_PSOLVE_FAIL_UNREC</code>, indicating that the preconditioner solve function <code>psolve</code> failed unrecoverably.</p> <p>If the CVSPTFQMR solve function failed (CVOICE returned <code>CV_LSOLVE_FAIL</code>), <code>lsflag</code> contains the error return flag from <code>SptfqmrSolve</code> and will be one of: <code>SPTFQMR_MEM_NULL</code>, indicating that the SPTFQMR memory is NULL; <code>SPTFQMR_ATIMES_FAIL_UNREC</code>, indicating an unrecoverable failure in the <math>J*v</math> function; or <code>SPTFQMR_PSOLVE_FAIL_UNREC</code>, indicating that the preconditioner solve function <code>psolve</code> failed unrecoverably.</p>	

#### 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.	

### 4.5.9 CVOICE reinitialization function

The function `CVOICEReInit` reinitializes the main CVOICE solver for the solution of a new problem, where a prior call to `CVOICEInit` been made. The new problem must have the same size as the previous one. `CVOICEReInit` performs the same input checking and initializations that `CVOICEInit` 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 `CV***` calls, 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 <code>CVODE</code> .
Arguments	<p><code>cvode_mem</code> (<code>void *</code>) pointer to the <code>CVODE</code> memory block.</p> <p><code>t0</code> (<code>realtype</code>) is the initial value of <math>t</math>.</p> <p><code>y0</code> (<code>N_Vector</code>) is the initial value of <math>y</math>.</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>CVodeReInit</code> was successful.</p> <p><code>CV_MEM_NULL</code> The <code>CVODE</code> memory block was not initialized through a previous call to <code>CVodeCreate</code>.</p> <p><code>CV_NO_MALLOC</code> Memory space for the <code>CVODE</code> memory block was not allocated through a previous call to <code>CVodeInit</code>.</p> <p><code>CV_ILL_INPUT</code> An input argument to <code>CVodeReInit</code> has an illegal value.</p>
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) a function that provides 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:

**CVRhsFn**

Definition	<pre>typedef int (*CVRhsFn)(realtype t, N_Vector y, N_Vector ydot,                         void *user_data);</pre>
Purpose	This function computes the ODE right-hand side for a given value of the independent variable $t$ and state vector $y$ .
Arguments	<p><math>t</math> is the current value of the independent variable.</p> <p><math>y</math> is the current value of the dependent variable vector, <math>y(t)</math>.</p> <p><math>ydot</math> is the output vector <math>f(t, y)</math>.</p> <p><math>user\_data</math> is the <code>user_data</code> pointer passed to <code>CVodeSetUserData</code>.</p>
Return value	A <code>CVRhsFn</code> should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and <code>CV_RHSFUNC_FAIL</code> is returned).
Notes	<p>Allocation of memory for <code>ydot</code> is handled within CVODE.</p> <p>A recoverable failure error return from the <code>CVRhsFn</code> is typically used to flag a value of the dependent variable <math>y</math> that is “illegal” in some way (e.g., negative where only a non-negative value is physically meaningful). If such a return is made, CVODE will attempt to recover (possibly repeating the Newton iteration, or reducing the step size) in order to avoid this recoverable error return.</p> <p>For efficiency reasons, the right-hand side function is not evaluated at the converged solution of the nonlinear solver. Therefore, in general, a recoverable error in that converged value cannot be corrected. (It may be detected when the right-hand side function is called the first time during the following integration step, but a successful step cannot be undone.)</p> <p>There are two other situations in which recovery is not possible even if the right-hand side function returns a recoverable error flag. One is when this occurs at the very first call to the <code>CVRhsFn</code> (in which case CVODE returns <code>CV_FIRST_RHSFUNC_ERR</code>). The other is when a recoverable error is reported by <code>CVRhsFn</code> after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODE returns <code>CV_UNREC_RHSFUNC_ERR</code>).</p>

#### 4.6.2 Error message handler function

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

**CVErrorHandlerFn**

Definition	<pre>typedef void (*CVErrorHandlerFn)(int error_code, const char *module,                                 const char *function, char *msg,                                 void *eh_data);</pre>
Purpose	This function processes error and warning messages from CVODE and its sub-modules.
Arguments	<p><code>error_code</code> is the error code.</p> <p><code>module</code> is the name of the CVODE module reporting the error.</p> <p><code>function</code> is the name of the function in which the error occurred.</p> <p><code>msg</code> is the error message.</p> <p><code>eh_data</code> is a pointer to user data, the same as the <code>eh_data</code> parameter passed to <code>CVodeSetErrHandlerFn</code>.</p>
Return value	A <code>CVErrorHandlerFn</code> function has no return value.
Notes	<code>error_code</code> is negative for errors and positive ( <code>CV_WARNING</code> ) for warnings. If a function that returns a pointer to memory encounters an error, it sets <code>error_code</code> to 0.

### 4.6.3 Error weight function

As an alternative to providing the relative and absolute tolerances, the user may provide a function of type `CVEwtFn` to compute a vector `ewt` containing the weights in the WRMS norm  $\|v\|_{\text{WRMS}} = \sqrt{(1/N) \sum_1^N (W_i \cdot v_i)^2}$ . These weights will be used in place of those defined by Eq. (2.6). The function type `CVEwtFn` is defined as follows:

**CVEwtFn**

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



### 4.6.4 Rootfinding function

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

**CVRootFn**

Definition	<pre>typedef int (*CVRootFn)(realtype t, N_Vector y, realtype *gout,                         void *user_data);</pre>
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	<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>gout</code> is the output array, of length <code>nrtfn</code> , with components $g_i(t,y)$ .
	<code>user_data</code> is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> .
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>CVODE</code> .

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

If the direct linear solver with dense treatment of the Jacobian is used (i.e., `CVDense` or `CVLapackDense` is called in Step 8 of §4.4), the user may provide a function of type `CVDlsDenseJacFn` defined by:

**CVDlsDenseJacFn**

**Definition**     `typedef (*CVDlsDenseJacFn)(long int N, realtype t, N_Vector y, N_Vector fy,  
     DlsMat Jac, void *user_data,  
     N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);`

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

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

**Return value** A `CVDlsDenseJacFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct, while CVDENSE sets `last_flag` to `CVDLS_JACFUNC_RECVR`), or a negative value if it failed unrecoverably (in which case the integration is halted, `CVode` returns `CV_LSETUP_FAIL` and CVDENSE sets `last_flag` to `CVDLS_JACFUNC_UNRECVR`).

**Notes**        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  $(t, y)$ . Only nonzero elements need to be loaded into `Jac` because `Jac` is set to the zero matrix before the call to the Jacobian function. The type of `Jac` is `DlsMat`.

The accessor macros `DENSE_ELEM` and `DENSE_COL` allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the `DlsMat` type. `DENSE_ELEM(J, i, j)` references the  $(i, j)$ -th element of the dense matrix `Jac` ( $i, j = 0 \dots N - 1$ ). 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 `DENSE_ELEM(J, m-1, n-1) = Jm,n`. Alternatively, `DENSE_COL(J, j)` returns a pointer to the first element of the  $j$ -th column of `Jac` ( $j = 0 \dots N - 1$ ), 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 = DENSE_COL(J, n-1); col_n[m-1] = Jm,n`. For large problems, it is more efficient to use `DENSE_COL` than to use `DENSE_ELEM`. Note that both of these macros number rows and columns starting from 0.

The `DlsMat` type and accessor macros `DENSE_ELEM` and `DENSE_COL` are documented in §8.1.3.

If the user's `CVDenseJacFn` function uses difference quotient approximations, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the `CVodeGet*` functions described in §4.5.8.1. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials.types.h`.

For the sake of uniformity, the argument  $N$  is of type `long int`, even in the case that the Lapack dense solver is to be used.

### 4.6.6 Jacobian information (direct method with banded Jacobian)

If the direct linear solver with banded treatment of the Jacobian is used (i.e. `CVBand` or `CVLapackBand` is called in Step 8 of §4.4), the user may provide a function of type `CVDlsBandJacFn` defined as follows:

<b>CVDlsBandJacFn</b>		
Definition	<pre>typedef int (*CVBandJacFn)(long int N, long int mupper, long int mlower,                            realtype t, N_Vector y, N_Vector fy,                            DlsMat Jac, void *user_data,                            N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);</pre>	
Purpose	This function computes the banded Jacobian $J = \partial f / \partial y$ (or a banded approximation to it).	
Arguments	N	is the problem size.
	mlower	
	mupper	are the lower and upper half-bandwidths of the Jacobian.
	t	is the current value of the independent variable.
	y	is the current value of the dependent variable vector, namely the predicted value of $y(t)$ .
	fy	is the current value of the vector $f(t, y)$ .
	Jac	is the output band Jacobian matrix (of type <code>DlsMat</code> ).
	user_data	is a pointer to user data, the same as the <code>user_data</code> parameter passed to <code>CVodeSetUserData</code> .
	tmp1	
	tmp2	
	tmp3	are pointers to memory allocated for variables of type <code>N_Vector</code> which can be used by <code>CVDlsBandJacFn</code> as temporary storage or work space.
Return value	A <code>CVDlsBandJacFn</code> function should return 0 if successful, a positive value if a recoverable error occurred (in which case <code>CVODE</code> will attempt to correct, while <code>CVBAND</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>CVode</code> returns <code>CV_LSETUP_FAIL</code> and <code>CVBAND</code> sets <code>last_flag</code> to <code>CVDLS_JACFUNC_UNRECVR</code> ).	
Notes	A user-supplied band Jacobian function must load the band matrix <code>Jac</code> of type <code>DlsMat</code> with the elements of the Jacobian $J(t, y)$ at the point $(t, y)$ . Only nonzero elements need to be loaded into <code>Jac</code> because <code>Jac</code> is initialized to the zero matrix before the call to the Jacobian function.	
	The accessor macros <code>BAND_ELEM</code> , <code>BAND_COL</code> , and <code>BAND_COL_ELEM</code> allow the user to read and write band matrix elements without making specific references to the underlying representation of the <code>DlsMat</code> type. <code>BAND_ELEM(J, i, j)</code> references the $(i, j)$ -th element of the band matrix <code>Jac</code> , 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 <code>mupper</code> and <code>mlower</code> , the Jacobian element $J_{m,n}$ can be loaded using the statement <code>BAND_ELEM(J, m-1, n-1) = J_{m,n}</code> . The elements within the band are those with $-\text{mupper} \leq m-n \leq \text{mlower}$ . Alternatively, <code>BAND_COL(J, j)</code> returns a pointer to the diagonal element of the $j$ -th column of <code>Jac</code> , and if we assign this address to <code>realtype *col_j</code> , then the $i$ -th element of the $j$ -th column is given by <code>BAND_COL_ELEM(col_j, i, j)</code> , counting from 0. Thus, for $(m, n)$ within the band, $J_{m,n}$ can be loaded by setting <code>col_n = BAND_COL(J, n-1)</code> ; <code>BAND_COL_ELEM(col_n, m-1, n-1) = J_{m,n}</code> . 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 <code>DlsMat</code> . The array <code>col_n</code> can be indexed from $-\text{mupper}$ to <code>mlower</code> . For large problems, it is more efficient to use <code>BAND_COL</code> and	

BAND\_COL\_ELEM than to use the BAND\_ELEM macro. As in the dense case, these macros all number rows and columns starting from 0.

The DlsMat type and the accessor macros BAND\_ELEM, BAND\_COL and BAND\_COL\_ELEM are documented in §8.1.4.

If the user's CVBandJacFn function uses difference quotient approximations, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` to `user_data` and then use the CVodeGet\* functions described in §4.5.8.1. The unit roundoff can be accessed as UNIT\_ROUNDOFF defined in `sundials_types.h`.

For the sake of uniformity, the arguments `N`, `mlower`, and `mupper` are of type `long int`, even in the case that the Lapack band solver is to be used.

#### 4.6.7 Jacobian information (direct method with sparse Jacobian)

If the direct linear solver with sparse treatment of the Jacobian is used (i.e., CVKLU or CVSuperLUMT is called in Step 8 of §4.4), the user must provide a function of type CVSlsSparseJacFn defined by:

CVSlsSparseJacFn
------------------

Definition	typedef (*CVSlsSparseJacFn)(realtype t, N_Vector y, N_Vector fy, SlsMat Jac, void *user_data, N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);		
Purpose	This function computes the sparse Jacobian $J = \partial f / \partial y$ (or an approximation to it).		
Arguments	t	is the current value of the independent variable.	
	y	is the current value of the dependent variable vector, namely the predicted value of $y(t)$ .	
	fy	is the current value of the vector $f(t, y)$ .	
	Jac	is the output sparse Jacobian matrix (of type SlsMat).	
	user_data	is a pointer to user data, the same as the user_data parameter passed to CVodeSetUserData.	
	tmp1 tmp2 tmp3	are pointers to memory allocated for variables of type N_Vector which can be used by a CVSlsSparseJacFn as temporary storage or work space.	
Return value	A CVSlsSparseJacFn should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct, while CVKLU or CVSUPERLUMT sets last_flag to CVSLS_JACFUNC_RECVR), or a negative value if it failed unrecoverably (in which case the integration is halted, CVode returns CV_LSETUP_FAIL and CVKLU or CVSUPERLUMT sets last_flag to CVSLS_JACFUNC_UNRECVR).		
Notes	<p>A user-supplied sparse Jacobian function must load the compressed-sparse-column matrix Jac with an approximation to the Jacobian matrix <math>J(t, y)</math> 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 row index arrays as needed. The type of Jac is SlsMat, and the amount of allocated space is available within the SlsMat structure as NNZ. The SlsMat type is further documented in the Section §8.2.</p> <p>If the user's CVSlsSparseJacFn function uses difference quotient approximations to set the specific nonzero matrix entries, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to cv_mem to user_data and then use</p>		

the `CNodeGet*` functions described in §4.5.8.1. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials.types.h`.

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

If one of the Krylov iterative linear solvers SPGMR, SPBCG, or SPTFQMR is selected (CVSp\* is called in step 8 of §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>CNodeSetUserData</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 to be 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>CNodeGet*</code> functions described in §4.5.8.1. The unit roundoff can be accessed as <code>UNIT_ROUNDOFF</code> defined in <code>sundials.types.h</code> .	

#### 4.6.9 Preconditioning (linear system solution)

If preconditioning is used, then the user must provide a `C` 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	<pre>typedef int (*CVSpilsPrecSolveFn)(realtype t, N_Vector y, N_Vector fy,                                    N_Vector r, N_Vector z,                                    realtype gamma, realtype delta,                                    int lr, void *user_data, N_Vector tmp);</pre>	
Purpose	This function solves the preconditioned system $Pz = r$ .	
Arguments	<code>t</code>	is the current value of the independent variable.
	<code>y</code>	is the current value of the dependent variable vector.

<b>fy</b>	is the current value of the vector $f(t, y)$ .
<b>r</b>	is the right-hand side vector of the linear system.
<b>z</b>	is the computed output vector.
<b>gamma</b>	is the scalar $\gamma$ appearing in the Newton matrix given by $M = I - \gamma J$ .
<b>delta</b>	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 <b>delta</b> in the weighted $l_2$ norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} < \mathbf{delta}$ . To obtain the <code>N_Vector ewt</code> , call <code>CVodeGetErrWeights</code> (see §4.5.8.1).
<b>lr</b>	is an input flag indicating whether the preconditioner solve function is to use the left preconditioner ( <b>lr</b> = 1) or the right preconditioner ( <b>lr</b> = 2);
<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to the function <code>CVodeSetUserData</code> .
<b>tmp</b>	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 to be returned by the preconditioner solve function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

#### 4.6.10 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 C function of type `CVSpilsPrecSetupFn`, defined as follows:

`CVSpilsPrecSetupFn`

<b>Definition</b>	<pre>typedef int (*CVSpilsPrecSetupFn)(realtype t, N_Vector y, N_Vector fy,                                    booleantype jok, booleantype *jcurPtr,                                    realtype gamma, void *user_data,                                    N_Vector tmp1, N_Vector tmp2,                                    N_Vector tmp3);</pre>														
<b>Purpose</b>	This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner.														
<b>Arguments</b>	<p>The arguments of a <code>CVSpilsPrecSetupFn</code> are as follows:</p> <table> <tr> <td><b>t</b></td><td>is the current value of the independent variable.</td></tr> <tr> <td><b>y</b></td><td>is the current value of the dependent variable vector, namely the predicted value of <math>y(t)</math>.</td></tr> <tr> <td><b>fy</b></td><td>is the current value of the vector <math>f(t, y)</math>.</td></tr> <tr> <td><b>jok</b></td><td>is an input flag indicating whether the Jacobian-related data needs to be updated. The <b>jok</b> argument provides for the reuse of Jacobian data in the preconditioner solve function. <b>jok</b> = <code>FALSE</code> means that the Jacobian-related data must be recomputed from scratch. <b>jok</b> = <code>TRUE</code> means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of <b>gamma</b>). A call with <b>jok</b> = <code>TRUE</code> can only occur after a call with <b>jok</b> = <code>FALSE</code>.</td></tr> <tr> <td><b>jcurPtr</b></td><td>is a pointer to a flag which should be set to <code>TRUE</code> if Jacobian data was recomputed, or set to <code>FALSE</code> if Jacobian data was not recomputed, but saved data was still reused.</td></tr> <tr> <td><b>gamma</b></td><td>is the scalar <math>\gamma</math> appearing in the Newton matrix <math>M = I - \gamma J</math>.</td></tr> <tr> <td><b>user_data</b></td><td>is a pointer to user data, the same as the <b>user_data</b> parameter passed to the function <code>CVodeSetUserData</code>.</td></tr> </table>	<b>t</b>	is the current value of the independent variable.	<b>y</b>	is the current value of the dependent variable vector, namely the predicted value of $y(t)$ .	<b>fy</b>	is the current value of the vector $f(t, y)$ .	<b>jok</b>	is an input flag indicating whether the Jacobian-related data needs to be updated. The <b>jok</b> argument provides for the reuse of Jacobian data in the preconditioner solve function. <b>jok</b> = <code>FALSE</code> means that the Jacobian-related data must be recomputed from scratch. <b>jok</b> = <code>TRUE</code> means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of <b>gamma</b> ). A call with <b>jok</b> = <code>TRUE</code> can only occur after a call with <b>jok</b> = <code>FALSE</code> .	<b>jcurPtr</b>	is a pointer to a flag which should be set to <code>TRUE</code> if Jacobian data was recomputed, or set to <code>FALSE</code> if Jacobian data was not recomputed, but saved data was still reused.	<b>gamma</b>	is the scalar $\gamma$ appearing in the Newton matrix $M = I - \gamma J$ .	<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to the function <code>CVodeSetUserData</code> .
<b>t</b>	is the current value of the independent variable.														
<b>y</b>	is the current value of the dependent variable vector, namely the predicted value of $y(t)$ .														
<b>fy</b>	is the current value of the vector $f(t, y)$ .														
<b>jok</b>	is an input flag indicating whether the Jacobian-related data needs to be updated. The <b>jok</b> argument provides for the reuse of Jacobian data in the preconditioner solve function. <b>jok</b> = <code>FALSE</code> means that the Jacobian-related data must be recomputed from scratch. <b>jok</b> = <code>TRUE</code> means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of <b>gamma</b> ). A call with <b>jok</b> = <code>TRUE</code> can only occur after a call with <b>jok</b> = <code>FALSE</code> .														
<b>jcurPtr</b>	is a pointer to a flag which should be set to <code>TRUE</code> if Jacobian data was recomputed, or set to <code>FALSE</code> if Jacobian data was not recomputed, but saved data was still reused.														
<b>gamma</b>	is the scalar $\gamma$ appearing in the Newton matrix $M = I - \gamma J$ .														
<b>user_data</b>	is a pointer to user data, the same as the <b>user_data</b> parameter passed to the function <code>CVodeSetUserData</code> .														

	<p>tmp1 tmp2 tmp3</p> <p>are pointers to memory allocated for variables of type <code>N_Vector</code> which can be used by <code>CVSpilsPrecSetupFn</code> as temporary storage or work space.</p>
Return value	The value to be returned by the preconditioner setup function is a flag indicating whether it was successful. This value should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).
Notes	<p>The operations performed by this function might include forming a crude approximate Jacobian, and performing an LU factorization of the resulting approximation to <math>M = I - \gamma J</math>.</p> <p>Each call to the preconditioner setup function is preceded by a call to the <code>CVRhsFn</code> user function with the same <math>(\mathbf{t}, \mathbf{y})</math> arguments. Thus, the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.</p> <p>This function is not called in advance of every call to the preconditioner solve function, but rather is called only as often as needed to achieve convergence in the Newton iteration.</p> <p>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 §4.5.8.1. The unit roundoff can be accessed as <code>UNIT_ROUNDOFF</code> defined in <code>sundials_types.h</code>.</p>

## 4.7 Preconditioner modules

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

### 4.7.1 A serial banded preconditioner module

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

In order to use the CVBANDPRE module, the user need not define any additional functions. Aside from the header files required for the integration of the ODE problem (see §4.3), to use the CVBANDPRE module, the main program must include the header file `cvode.bandpre.h` which declares the needed function prototypes. The following is a summary of the usage of this module. Steps that are unchanged from the skeleton program presented in §4.4 are grayed out.

1. Set problem dimensions
2. Set vector of initial values
3. Create CVODE object

## 4. Allocate internal memory

## 5. Set optional inputs

## 6. Attach iterative linear solver, one of:

- (a) `flag = CVSpqr(cvode_mem, pretype, maxl);`
- (b) `flag = CVSpbcg(cvode_mem, pretype, maxl);`
- (c) `flag = CVSptfqmr(cvode_mem, pretype, maxl);`

## 7. 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.

## 8. Set linear solver optional inputs

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

## 9. Advance solution in time

## 10. Get optional outputs

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

## 11. Deallocate memory for solution vector

## 12. Free solver memory

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

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

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

Description The function `CVBandPrecInit` initializes the CVBANDPRE preconditioner and allocates required (internal) memory for it.

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

`N` (long int) problem dimension.

`mu` (long int) upper half-bandwidth of the Jacobian approximation.

`m1` (long int) lower half-bandwidth of the Jacobian approximation.

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

`CVSPILS_SUCCESS` The call to `CVBandPrecInit` 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 memory was not attached.

`CVSPILS_ILL_INPUT` The supplied vector implementation was not compatible with block band preconditioner.

Notes The banded approximate Jacobian will have nonzero elements only in locations  $(i, j)$  with  $-m1 \leq j - i \leq mu$ .

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

**CVBandPrecGetWorkSpace**

Call	<code>flag = CVBandPrecGetWorkSpace(cvode_mem, &amp;lenrwBP, &amp;leniwBP);</code>
Description	The function <code>CVBandPrecGetWorkSpace</code> returns the sizes of the CVBANDPRE real and integer workspaces.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>lenrwBP</code> (long int) the number of <code>realtype</code> values in the CVBANDPRE workspace. <code>leniwBP</code> (long int) the number of integer values in the CVBANDPRE workspace.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of: <code>CVSPILS_SUCCESS</code> The optional output values have been successfully set. <code>CVSPILS_PMEM_NULL</code> The CVBANDPRE preconditioner has not been initialized.
Notes	<p>In terms of problem size <math>N</math> and <math>\text{smu} = \min(N - 1, \text{mu} + \text{ml})</math>, the actual size of the real workspace is <math>(2 \text{ml} + \text{mu} + \text{smu} + 2) N</math> <code>realtype</code> words, and the actual size of the integer workspace is <math>N</math> integer words.</p> <p>The workspaces referred to here exist in addition to those given by the corresponding function <code>CVSpils***GetWorkSpace</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 finite difference banded Jacobian approximation used within the preconditioner setup function.
Arguments	<code>cvode_mem</code> (void *) pointer to the CVODE memory block. <code>nfevalsBP</code> (long int) the number of calls to the user right-hand side function.
Return value	The return value <code>flag</code> (of type <code>int</code> ) is one of: <code>CVSPILS_SUCCESS</code> The optional output value has been successfully set. <code>CVSPILS_PMEM_NULL</code> The CVBANDPRE preconditioner has not been initialized.
Notes	The counter <code>nfevalsBP</code> is distinct from the counter <code>nfevalsLS</code> returned by the corresponding function <code>CVSpils***GetNumRhsEvals</code> , and also from <code>nfevals</code> , returned by <code>CVodeGetNumRhsEvals</code> . The total number of right-hand side function evaluations is the sum of all three of these counters.

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

A principal reason for using a parallel ODE solver such as CVODE lies in the solution of partial differential equations (PDEs). Moreover, the use of a Krylov iterative method for the solution of many such problems is motivated by the nature of the underlying linear system of equations (2.4) 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 [21] and is included in a software module within the CVODE package. This module works with the parallel vector module `NVECTOR_PARALLEL` and is usable with any of the Krylov iterative linear solvers. 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)(long int 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.	

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

- Return value A `CVLocalFn` should return 0 if successful, a positive value if a recoverable error occurred (in which case `CVODE` will attempt to correct), or a negative value if it failed unrecoverably (in which case the integration is halted and `CVode` returns `CV_LSETUP_FAIL`).
- Notes This function must assume that all interprocess communication of data needed to calculate `glocal` has already been done, and that this data is accessible within `user_data`. The case where  $g$  is mathematically identical to  $f$  is allowed.

#### CVCommFn

- Definition 

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

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

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

1. Initialize MPI
2. Set problem dimensions
3. Set vector of initial values
4. Create `CVODE` object
5. Allocate internal memory
6. Set optional inputs
7. Attach iterative linear solver, one of:
  - (a) `flag = CVSpgrmr(cvode_mem, pretype, maxl);`
  - (b) `flag = CVSpbcg(cvode_mem, pretype, maxl);`
  - (c) `flag = CVSpTFqmr(cvode_mem, pretype, maxl);`

```
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);
```

## 9. Set linear solver optional inputs

## 10. Advance solution in time

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

### 13. Free solver memory

The user-callable functions that initialize (step 8 above) or re-initialize the CVBBDPRE preconditioner module are described next.

[illegible]

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

`local_N` (long int) local vector length.

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

**mlldq** (long int) lower half-bandwidth to be used in the difference quotient Jacobian approximation.

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

**mlkeep** (long int) 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** (CVCCommFn) the optional C function which performs all interprocess communication required for the computation of  $q(t, y)$ .

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

CVSPILS\_SUCCESS    The call to CVBBDPrecInit was successful.

CVSPILS\_MEM\_NULL The `cnode_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 CVODE for a subsequent problem, a call to `CVBBDPrecReInit` can be made to change any of the following: the half-bandwidths `mudq` and `mldq` used in the difference-quotient Jacobian approximations, the relative increment `dqrely`, or one of the user-supplied functions `gloc` and `cfn`. If there is a change in any of the linear solver inputs, an additional call to `CVSpgmr`, `CVSpbcg`, or `CVSptfqmr`, and/or one or more of the corresponding `CVSpils***Set***` functions, must also be made (in the proper order).

#### CVBBDPrecReInit

Call `flag = CVBBDPrecReInit(cvode_mem, mudq, mldq, dqrely);`  
 Description The function `CVBBDPrecReInit` re-initializes the CVBBDPRE preconditioner.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `mudq` (long int) upper half-bandwidth to be used in the difference quotient Jacobian approximation.  
           `mldq` (long int) lower half-bandwidth to be used in the difference quotient Jacobian approximation.  
           `dqrely` (realtype) the relative increment in components of  $y$  used in the difference quotient approximations. The default is `dqrely =  $\sqrt{\text{unit roundoff}}$` , which can be specified by passing `dqrely = 0.0`.

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

CVSPILS\_SUCCESS The call to `CVBBDPrecReInit` was successful.  
 CVSPILS\_MEM\_NULL The `cvode_mem` pointer was NULL.  
 CVSPILS\_LMEM\_NULL A CVSPILS linear solver memory was not attached.  
 CVSPILS\_PMEM\_NULL The function `CVBBDPrecInit` was not previously called.

Notes If one of the half-bandwidths `mudq` or `mldq` is negative or exceeds the value `local_N-1`, it is replaced by 0 or `local_N-1` accordingly.

The following two optional output functions are available for use with the CVBBDPRE module:

#### CVBBDPrecGetWorkSpace

Call `flag = CVBBDPrecGetWorkSpace(cvode_mem, &lenrwBBDP, &leniwBBDP);`  
 Description The function `CVBBDPrecGetWorkSpace` returns the local CVBBDPRE real and integer workspace sizes.  
 Arguments `cvode_mem` (void \*) pointer to the CVODE memory block.  
           `lenrwBBDP` (long int) local number of `realtype` values in the CVBBDPRE workspace.

	<code>leniwBBDP</code> ( <code>long int</code> ) local number of integer values in the CVBBDPRE workspace.
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 output value has been successfully set.</li> <li><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.</li> <li><code>CVSPILS_PMEM_NULL</code> The CVBBDPRE preconditioner has not been initialized.</li> </ul>
Notes	In terms of <code>local_N</code> and <code>smu = min(local_N - 1, mukeep + mlkeep)</code> , the actual size of the real workspace is $(2 \text{ mlkeep} + \text{mukeep} + \text{smu} + 2) \text{ local\_N realtype}$ words, and the actual size of the integer workspace is <code>local_N</code> integer words. These values are local to each process.  The workspaces referred to here exist in addition to those given by the corresponding function <code>CVSpils***GetWorkSpace</code> .

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	<code>cvode_mem</code> ( <code>void *</code> ) pointer to the CVOICE memory block. <code>ngevalsBBDP</code> ( <code>long int</code> ) the number of calls made to the user-supplied <code>gloc</code> function.
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 output value has been successfully set.</li> <li><code>CVSPILS_MEM_NULL</code> The <code>cvode_mem</code> pointer was NULL.</li> <li><code>CVSPILS_PMEM_NULL</code> The CVBBDPRE preconditioner has not been initialized.</li> </ul>

In addition to the `ngevalsBBDP` `gloc` evaluations, the costs associated with CVBBDPRE also include `nlinsetups` LU factorizations, `nlinsetups` calls to `cfn`, `npsolves` banded backsolve calls, and `nfevalsLS` right-hand side function evaluations, where `nlinsetups` is an optional CVOICE output and `npsolves` and `nfevalsLS` are linear solver optional outputs (see §4.5.8).

## Chapter 5

# FCVODE, an Interface Module for FORTRAN Applications

The FCVODE interface module is a package of C functions which support the use of the CVODE solver, for the solution of ODE systems  $dy/dt = f(t, y)$ , in a mixed FORTRAN/C setting. While CVODE is written in C, it is assumed here that the user's calling program and user-supplied problem-defining routines are written in FORTRAN. This package provides the necessary interface to CVODE for all supplied serial and parallel NVECTOR implementations.

### 5.1 Important note on portability

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

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

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

### 5.2 Fortran Data Types

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

**Integers:** SUNDIALS uses both `int` and `long int` types:

- `int` – equivalent to an `INTEGER` or `INTEGER*4` in FORTRAN
- `long int` – this will depend on the computer architecture:
  - 32-bit architecture – equivalent to an `INTEGER` or `INTEGER*4` in FORTRAN
  - 64-bit architecture – equivalent to an `INTEGER*8` in FORTRAN

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

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

## 5.3 FCVODE routines

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

- Interface to the NVECTOR modules
  - `FNVINITS` (defined by `NVECTOR_SERIAL`) interfaces to `N_VNewEmpty_Serial`.
  - `FNVINITP` (defined by `NVECTOR_PARALLEL`) interfaces to `N_VNewEmpty_Parallel`.
  - `FNVINITOMP` (defined by `NVECTOR_OPENMP`) interfaces to `N_VNewEmpty_OpenMP`.
  - `FNVINITPTS` (defined by `NVECTOR_PTHREADS`) interfaces to `N_VNewEmpty_Pthreads`.
- Interface to the main CVOID module
  - `FCVMALLOC` interfaces to `CVodeCreate`, `CVodeSetUserData`, and `CVodeInit`, as well as one of `CVodeSStolerances` or `CVodeSVtolerances`.
  - `FCVREINIT` interfaces to `CVodeReInit`.
  - `FCVSETIIN` and `FCVSETRIN` interface to `CVodeSet*` functions.
  - `FCVEWTSET` interfaces to `CVodeWftolerances`.
  - `FCVODE` interfaces to `CVode`, `CVodeGet*` functions, and to the optional output functions for the selected linear solver module.
  - `FCVDKY` interfaces to the interpolated output function `CVodeGetDky`.
  - `FCVGETERRWEIGHTS` interfaces to `CVodeGetErrWeights`.
  - `FCVGETESTLOCALERR` interfaces to `CVodeGetEstLocalErrors`.
  - `FCVFREE` interfaces to `CVodeFree`.
- Interface to the linear solver modules
  - `FCVDIAG` interfaces to `CVDiag`.
  - `FCVDENSE` interfaces to `CVDense`.
  - `FCVDENSESETJAC` interfaces to `CVDlsSetDenseJacFn`.
  - `FCVLAPACKDENSE` interfaces to `CVLapackDense`.
  - `FCVLAPACKDENSESETJAC` interfaces to `CVDlsSetDenseJacFn`.
  - `FCVBAND` interfaces to `CVBand`.
  - `FCVBANDSETJAC` interfaces to `CVDlsSetBandJacFn`.
  - `FCVLAPACKBAND` interfaces to `CVLapackBand`.
  - `FCVLAPACKBANDSETJAC` interfaces to `CVDlsSetBandJacFn`.
  - `FCVKLU` interfaces to `CVKLU`.
  - `FCVKLUREINIT` interfaces to `CVKLUREInit`.
  - `FCVSUPERLUMT` interfaces to `CVSuperLUMT`.

- FCVSPARSESETJAC interfaces to `CVSlsSetSparseJacFn`.
- FCVSPGMR interfaces to `CVSpgm` and SPGMR optional input functions.
- FCVSPGMRREINIT interfaces to SPGMR optional input functions.
- FCVSPBCG interfaces to `CVSpbcg` and SPBCG optional input functions.
- FCVSPBCGREINIT interfaces to SPBCG optional input functions.
- FCVSPTFQMR interfaces to `CVSptfqmr` and SPTFQMR optional input functions.
- FCVSPTFQMRREINIT interfaces to SPTFQMR optional input functions.
- FCVSPILSSETJAC interfaces to `CVSpilsSetJacTimesVecFn`.
- FCVSPILSSETPREC interfaces to `CVSpilsSetPreconditioner`.

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

FCVODE routine (FORTRAN, user-supplied)	CVODE function (C, interface)	CVODE type of interface function
FCVFUN	FCVf	CVRhsFn
FCVEWT	FCVEwtSet	CVWEwtFn
FCVDJAC	FCVDenseJac	CVDlsDenseJacFn
	FCVLapackDenseJac	CVDlsDenseJacFn
FCVBjac	FCVBandJac	CVDlsBandJacFn
	FCVLapackBandJac	CVDlsBandJacFn
FCVSPJAC	FCVSparsJac	CVSlsSparseJacFn
FCVPSOL	FCVPSol	CVSpilsPrecSolveFn
FCVPSET	FCVPSet	CVSpilsPrecSetupFn
FCVJTURNS	FCVJtimes	CVSpilsJacTimesVecFn

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

## 5.4 Usage of the FCVODE interface module

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

### 1. Right-hand side specification

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

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

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

## 2. NVECTOR module initialization

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

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

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

## 3. Problem specification

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

FCVMALLOC
-----------

Call	CALL FCVMALLOC(TO, YO, METH, ITMETH, IATOL, RTOL, ATOL, & IOUT, ROUT, IPAR, RPAR, IER)
Description	This function provides required problem and solution specifications, specifies optional inputs, allocates internal memory, and initializes CVODE.
Arguments	<p>TO is the initial value of <math>t</math>.</p> <p>YO is an array of initial conditions.</p> <p>METH specifies the basic integration method: 1 for Adams (nonstiff) or 2 for BDF (stiff).</p> <p>ITMETH specifies the nonlinear iteration method: 1 for functional iteration or 2 for Newton iteration.</p> <p>IATOL specifies the type for absolute tolerance ATOL: 1 for scalar or 2 for array. If IATOL= 3, the arguments RTOL and ATOL are ignored and the user is expected to subsequently call FCVEWTSET and provide the function FCVEWT.</p> <p>RTOL is the relative tolerance (scalar).</p> <p>ATOL is the absolute tolerance (scalar or array).</p> <p>IOUT is an integer array of length 21 for integer optional outputs.</p> <p>ROUT is a real array of length 6 for real optional outputs.</p> <p>IPAR is an integer array of user data which will be passed unmodified to all user-provided routines.</p> <p>RPAR is a real array of user data which will be passed unmodified to all user-provided routines.</p>
Return value	IER is a return completion flag. Values are 0 for successful return and $-1$ otherwise. See printed message for details in case of failure.
Notes	<p>The user integer data arrays IOUT and IPAR must be declared as INTEGER*4 or INTEGER*8 according to the C type long int.</p> <p>Modifications to the user data arrays IPAR and RPAR inside a user-provided routine will be propagated to all subsequent calls to such routines.</p> <p>The optional outputs associated with the main CVODE integrator are listed in Table 5.2.</p>

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

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

It must set the positive components of the error weight vector EWT for the calculation of the WRMS norm of Y. On return, set IER = 0 if FCVEWT was successful, and nonzero otherwise. The

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

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

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

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

#### 4. Set optional inputs

Call `FCVINSETIIN` and/or `FCVINSETRIN` to set desired optional inputs, if any. See §5.5 for details.

#### 5. Linear solver specification

In the case of a stiff system, the implicit BDF method involves the solution of linear systems related to the Jacobian  $J = \partial f / \partial y$  of the ODE system. The user of FCVODE must call a routine with a specific name to make the desired choice of linear solver. Note that the direct (dense or band) and sparse linear solver options are usable only in a serial environment.

##### Diagonal approximate Jacobian

This choice is appropriate when the Jacobian can be well approximated by a diagonal matrix. The user must make the call:

```
CALL FCVDIAG(IER)
```

`IER` is an error return flag set on 0 on success or  $-1$  if a memory failure occurred. There is no additional user-supplied routine. Optional outputs specific to the `DIAG` case listed in Table 5.2.

##### Dense treatment of the linear system

To use the direct dense linear solver based on the internal CVIDE implementation, the user must make the call:

```
CALL FCVDENSE(NEQ, IER)
```

where `NEQ` is the size of the ODE system. The argument `IER` is an error return flag which is 0 for success,  $-1$  if a memory allocation failure occurred, or  $-2$  for illegal input.

Alternatively, to use the Lapack-based direct dense linear solver, the user must make the call:

```
CALL FCVLAPACKDENSE(NEQ, IER)
```

where the arguments have the same meanings as for `FCVDENSE`, except that here `NEQ` must be declared so as to match C type `int`.

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

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

Typically this routine will use only `NEQ`, `T`, `Y`, and `DJAC`. It must compute the Jacobian and store it columnwise in `DJAC`. The input arguments `T`, `Y`, and `FY` contain the current values of  $t$ ,  $y$ , and

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

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

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

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

with `FLAG`  $\neq 0$  to specify use of the user-supplied Jacobian approximation. The argument `IER` is an error return flag which is 0 for success or non-zero if an error occurred. If using the Lapack-based direct dense linear solver, the use of a Jacobian approximation supplied by the user is indicated through the call

```
CALL FCVLAPACKDENSESETJAC (FLAG, IER)
```

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

### Band treatment of the linear system

To use the direct band linear solver based on the internal `CVODE` implementation, the user must make the call:

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

The arguments are: `MU`, the upper half-bandwidth; `ML`, the lower half-bandwidth; and `IER` an error return flag which is 0 for success,  $-1$  if a memory allocation failure occurred, or  $-2$  in case an input has an illegal value.

Alternatively, to use the Lapack-based direct band linear solver, the user must make the call:

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

where the arguments have the same meanings as for `FCVBAND`, except that here `NEQ`, `MU`, and `ML` must be declared so as to match C type `int`.

As an option when using the `BAND` linear solver, the user may supply a routine that computes a band approximation of the system Jacobian  $J = \partial f / \partial y$ . If supplied, it must have the following form:

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

Typically this routine will use only `NEQ`, `MU`, `ML`, `T`, `Y`, and `BJAC`. It must load the `MDIM` by `N` array `BJAC` with the Jacobian matrix at the current  $(t, y)$  in band form. Store in `BJAC(k, j)` the

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

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

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

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

with **FLAG**  $\neq 0$  to specify use of the user-supplied Jacobian approximation. The argument **IER** is an error return flag which is 0 for success or non-zero if an error occurred. If using the Lapack-based direct band linear solver, the use of a Jacobian approximation supplied by the user is indicated through the call

```
CALL FCVLAPACKNBANDSETJAC (FLAG, IER)
```

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

### Sparse direct treatment of the linear system

To use the **KLU** sparse direct linear solver, the user must make the call:

```
CALL FCVKLU (NEQ, NNZ, SPARSETYPE, ORDERING, IER)
```

where **NEQ** is the size of the ODE system, **NNZ** is the maximum number of nonzeros in the Jacobian matrix, **SPARSETYPE** is a flag indicating whether the matrix is in compressed-sparse-column or compressed-sparse-row format (0 = **CSC**, 1 = **CSR**), and **ORDERING** is the matrix ordering desired with possible values from the **KLU** package (0 = **AMD**, 1 = **COLAMD**). The argument **IER** is an error return flag which is 0 for success or negative for an error.

The **CVODE KLU** solver will reuse much of the factorization information from one nonlinear iteration and time step to the next. If at any time the user wants to force a full refactorization, or if the number of nonzeros in the Jacobian matrix changes, the user should make the call

```
CALL FCVKLUREINIT(NEQ, NNZ, REINIT_TYPE)
```

where **NEQ** is the size of the ODE system, **NNZ** is the maximum number of nonzeros in the Jacobian matrix, and **REINIT\_TYPE** is 1 or 2. For a value of 1, the matrix will be destroyed and a new one will be allocated with **NNZ** nonzeros. For a value of 2, only symbolic and numeric factorizations will be completed.

Alternatively, to use the **SuperLUMT** linear solver, the user must make the call:

```
CALL FCVSUPERLUMT (NTHREADS, NEQ, NNZ, ORDERING, IER)
```

where `NTHREADS` is the number of threads requested and the other arguments have the same meanings as for `FCVKLU`, except that here possible values for `ORDERING` derive from the `SUPERLUMT` package and include: 0 for Natural ordering, 1 for Minimum degree on  $A^T A$ , 2 for Minimum degree on  $A^T + A$ , and 3 for COLAMD.

If either of the sparse direct interface packages are used, then the user must supply the `FCVSPJAC` routine that computes a compressed-sparse-column [or compressed-sparse-row if using `KLU`] approximation of the system Jacobian  $J = \partial f / \partial y$ . If supplied, it must have the following form:

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

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

To indicate that the `FCVSPJAC` routine has been provided, then following either the call to `FCVKLU` or `FCVSUPERLUMT`, the following call must be made

```
CALL FCVSPARSESETJAC (IER)
```

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

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

### SPGMRES treatment of the linear systems

For the Scaled Preconditioned GMRES solution of the linear systems, the user must make the call

```
CALL FCVSPGMRES(IPRETYPE, IGSTYPE, MAXL, DELT, IER)
```

The arguments are as follows. `IPRETYPE` specifies the preconditioner type: 0 for no preconditioning, 1 for left only, 2 for right only, or 3 for both sides. `IGSTYPE` indicates the Gram-Schmidt process type: 1 for modified G-S or 2 for classical G-S. `MAXL` is the maximum Krylov subspace dimension. `DELT` is the linear convergence tolerance factor. For all of the input arguments, a value of 0 or 0.0 indicates the default. `IER` is an error return flag which is 0 to indicate success,  $-1$  if a memory allocation failure occurred, or  $-2$  to indicate an illegal input.

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

For descriptions of the relevant optional user-supplied routines, see **User-supplied routines for SPGMRES/SPBCG/SPTFQMR** below.

### SPBCG treatment of the linear systems

For the Scaled Preconditioned Bi-CGStab solution of the linear systems, the user must make the call

```
CALL FCVSPBCG(IPRETYPE, MAXL, DELT, IER)
```

Its arguments are the same as those with the same names for FCVSPGMR.

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

For descriptions of the relevant optional user-supplied routines, see **User-supplied routines for SPGMR/SPBCG/SPTFQMR** below.

#### **SPTFQMR treatment of the linear systems**

For the Scaled Preconditioned Transpose-Free Quasi-Minimal Residual solution of the linear systems, the user must make the call

```
CALL FCVSPTFQMR(IPRETYPE, MAXL, DELT, IER)
```

Its arguments are the same as those with the same names for FCVSPGMR.

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

For descriptions of the relevant optional user-supplied routines, see below.

#### **Functions used by SPGMR/SPBCG/SPTFQMR**

An optional user-supplied routine, FCVJTIMES (see below), can be provided for Jacobian-vector products. If it is, then, following the call to FCVSPGMR, FCVSPBCG, or FCVSPTFQMR, the user must make the call:

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

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

If preconditioning is to be done ( $\text{IPRETYPE} \neq 0$ ), then the user must call

```
CALL FCVSPILSSETPREC(FLAG, IER)
```

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

#### **User-supplied routines for SPGMR/SPBCG/SPTFQMR**

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

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

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

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

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

```

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

```

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

The arrays  $IPAR$  (of integers) and  $RPAR$  (of reals) contain user data and are the same as those passed to FCVMALLOC. The argument  $WORK$  is a work array of length  $NEQ$  for use by this routine.

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

```

SUBROUTINE FCVPSET(T, Y, FY, JOK, JCUR, GAMMA, H, IPAR, RPAR,
&                WORK1, WORK2, WORK3, IER)
  DIMENSION Y(*), FY(*), EWT(*), IPAR(*), RPAR(*),
&                WORK1(*), WORK2(*), WORK3(*)

```

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

The arrays  $IPAR$  (of integers) and  $RPAR$  (of reals) contain user data and are the same as those passed to FCVMALLOC. The arguments  $WORK1$ ,  $WORK2$ ,  $WORK3$  are work arrays of length  $NEQ$  for use by this routine.



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

## Notes

- (a) If the user's FCVJTIMES or FCVPSET routine uses difference quotient approximations, it may need to use the error weight array  $EWT$ , the current stepsize  $H$ , and/or the unit roundoff, in the calculation of suitable increments. Also, If FCVPSOL uses an iterative method in its solution, the residual vector  $\rho = r - Pz$  of the system should be made less than  $DELTA$  in weighted  $\ell_2$  norm, i.e.  $\sqrt{\sum (\rho_i * EWT[i])^2} < DELTA$ .
- (b) If needed in FCVJTIMES, FCVPSOL, or FCVPSET, the error weight array  $EWT$  can be obtained by calling FCVGETERRWEIGHTS using one of the work arrays as temporary storage for  $EWT$ .
- (c) If needed in FCVJTIMES, FCVPSOL, or FCVPSET, the unit roundoff can be obtained as the optional output  $ROUT(6)$  (available after the call to FCVMALLOC) and can be passed using either the  $RPAR$  user data array or a common block.

## 6. Problem solution

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

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

The arguments are as follows. TOUT specifies the next value of  $t$  at which a solution is desired (input). T is the value of  $t$  reached by the solver on output. Y is an array containing the computed solution on output. ITASK is a task indicator and should be set to 1 for normal mode (overshoot TOUT and interpolate), or to 2 for one-step mode (return after each internal step taken). IER is a completion flag and will be set to a positive value upon successful return or to a negative value if an error occurred. These values correspond to the CVode returns (see §4.5.5 and §B.2). The current values of the optional outputs are available in IOUT and ROUT (see Table 5.2).

## 7. Additional solution output

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

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

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

## 8. Problem reinitialization

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

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

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

Following this call, a call to specify the linear system solver must be made if the choice of linear solver is being changed. Otherwise, a call to reinitialize the linear solver last used may or may not be needed, depending on changes in the inputs to it.

In the case of the BAND solver, for any change in the half-bandwidth parameters, call FCVBAND (or FCVLAPACKBAND) as described above.

In the case of SPGMR, for a change of inputs other than MAXL, make the call

```
CALL FCVSPGMRREINIT (IPRETYPE, IGSTYPE, DELT, IER)
```

which reinitializes SPGMR without reallocating its memory. The arguments have the same names and meanings as those of FCVSPGMR. If MAXL is being changed, then call FCVSPGMR instead.

In the case of SPBCG, for a change in any inputs, make the call

```
CALL FCVSPBCGREINIT (IPRETYPE, MAXL, DELT, IER)
```

which reinitializes SPBCG without reallocating its memory. The arguments have the same names and meanings as those of FCVSPBCG.

In the case of SPTFQMR, for a change in any inputs, make the call

```
CALL FCVSPTFQMRREINIT (IPRETYPE, MAXL, DELT, IER)
```

which reinitializes SPTFQMR without reallocating its memory. The arguments have the same names and meanings as those of FCVSPTFQMR.

Table 5.1: Keys for setting FCVODE optional inputs

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

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

## 9. Memory deallocation

To free the internal memory created by the call to FCVMALLOC, make the call

```
CALL FCVFREE
```

## 5.5 FCVODE optional input and output

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

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

where **KEY** is a quoted string indicating which optional input is set (see Table 5.1), **IVAL** is the integer input value to be used, **RVAL** is the real input value to be used, and **IER** is an integer return flag which is set to 0 on success and a negative value if a failure occurred. The integer **IVAL** should be declared in a manner consistent with C type `long int`.

The optional outputs from the CVODE solver are accessed not through individual functions, but rather through a pair of arrays, **IOUT** (integer type) of dimension at least 21, and **ROUT** (real type) of dimension at least 6. These arrays are owned (and allocated) by the user and are passed as arguments to FCVMALLOC. Table 5.2 lists the entries in these two arrays and specifies the optional variable as well as the CVODE function which is actually called to extract the optional output.

For more details on the optional inputs and outputs, see §4.5.6 and §4.5.8.

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

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

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

This computes the **EWT** array normally defined by Eq. (2.6). The array **EWT**, of length **NEQ** or **NLOCAL**, must already have been declared by the user. The error return flag **IER** is zero if successful, and negative if there was a memory error.

Table 5.2: Description of the FCVODE optional output arrays IOU and ROUT

Integer output array IOU		
Index	Optional output	CVODE function
CVODE main solver		
1	LENRW	CVodeGetWorkSpace
2	LENIW	CVodeGetWorkSpace
3	NST	CVodeGetNumSteps
4	NFE	CVodeGetNumRhsEvals
5	NETF	CVodeGetNumErrTestFails
6	NCFN	CVodeGetNumNonlinSolvConvFails
7	NNI	CVodeGetNumNonlinSolvIters
8	NSETUPS	CVodeGetNumLinSolvSetups
9	QU	CVodeGetLastOrder
10	QCUR	CVodeGetCurrentOrder
11	NOR	CVodeGetNumStabLimOrderReds
12	NGE	CVodeGetNumGEvals
CVDLS linear solvers		
13	LENRWLS	CVDlsGetWorkSpace
14	LENIWLS	CVDlsGetWorkSpace
15	LS_FLAG	CVDlsGetLastFlag
16	NFELS	CVDlsGetNumRhsEvals
17	NJE	CVDlsGetNumJacEvals
CVDIAG linear solver		
13	LENRWLS	CVDdiagGetWorkSpace
14	LENIWLS	CVDdiagGetWorkSpace
15	LS_FLAG	CVDdiagGetLastFlag
16	NFELS	CVDdiagGetNumRhsEvals
CVSLS linear solvers		
14	LS_FLAG	CVSlsGetLastFlag
16	NJE	CVSlsGetNumJacEvals
CVSPILS linear solvers		
13	LENRWLS	CVSpilsGetWorkSpace
14	LENIWLS	CVSpilsGetWorkSpace
15	LS_FLAG	CVSpilsGetLastFlag
16	NFELS	CVSpilsGetNumRhsEvals
17	NJTV	CVSpilsGetNumJacEvals
18	NPE	CVSpilsGetNumPrecEvals
19	NPS	CVSpilsGetNumPrecSolves
20	NLI	CVSpilsGetNumLinIters
21	NCFL	CVSpilsGetNumConvFails

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

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

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

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

## 5.6 Usage of the FCVROOT interface to rootfinding

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

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

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

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

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

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

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

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

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

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

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

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

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

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

```
CALL FCVROOTFREE
```

## 5.7 Usage of the FCVBP interface to CVBANDPRE

The FCVBP interface sub-module is a package of C functions which, as part of the FCVODE interface module, support the use of the CVODE solver with the serial NVECTOR\_SERIAL module, and the combination of the CVBANDPRE preconditioner module (see §4.7.1) with any of the Krylov iterative linear solvers.

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

- FCVBPINIT interfaces to CVBandPrecInit.
- FCVBPOPT interfaces to CVBANDPRE optional output functions.

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

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

1. Right-hand side specification
2. NVECTOR module initialization
3. Problem specification
4. Set optional inputs
5. Linear solver specification

First, specify one of the CVSPILS iterative linear solvers, by calling one of FCVSPGMR, FCVSPBCG, or FCVSPTFQMR.

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

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

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

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

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

with `FLAG`  $\neq 0$  (see step 5 in §5.4 for details).

6. Problem solution
7. CVBANDPRE Optional outputs

Optional outputs specific to the SPGMR, SPBCG, or SPTFQMR solver are listed in Table 5.2. To obtain the optional outputs associated with the CVBANDPRE module, make the following call:

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

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

## 8. Memory deallocation

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

## 5.8 Usage of the FCVBBD interface to CVBBDPRE

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

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

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

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

FCVBBD routine (FORTRAN, user-supplied)	CVODE function (C, interface)	CVODE type of interface function
FCVLOCFN	FCVgloc	CVLocalFn
FCVCOMMF	FCVcfn	CVCommFn
FCVJTIMES	FCVJtimes	CVSpilsJacTimesVecFn

As with the rest of the FCVODE routines, the names of all user-supplied routines here are fixed, in order to maximize portability for the resulting mixed-language program. Additionally, based on flags discussed above in §5.3, the names of the user-supplied routines are mapped to actual values through a series of definitions in the header file `fcvbdd.h`.

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

1. **Right-hand side specification**
2. **NVECTOR module initialization**
3. **Problem specification**
4. **Set optional inputs**
5. **Linear solver specification**

First, specify one of the CVSPILS iterative linear solvers, by calling one of FCVSPGMR, FCVSPBCG, or FCVSPTFQMR.

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

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

The arguments are as follows. `NLOCAL` is the local size of vectors on this processor. `MUDQ` and `MLDQ` are the upper and lower half-bandwidths to be used in the computation of the local Jacobian blocks by difference quotients. These may be smaller than the true half-bandwidths of the Jacobian of the local block of  $g$ , when smaller values may provide greater efficiency. `MU` and `ML` are the upper and lower half-bandwidths of the band matrix that is retained as an approximation of the local

Jacobian block. These may be smaller than MUDQ and MLDQ. DQRELY is the relative increment factor in  $y$  for difference quotients (optional). A value of 0.0 indicates the default,  $\sqrt{\text{unit roundoff}}$ . IER is a return completion flag. A value of 0 indicates success, while a value of  $-1$  indicates that a memory failure occurred or that an input had an illegal value.

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

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

with  $\text{FLAG} \neq 0$  (see step 5 in §5.4 for details).

## 6. Problem solution

### 7. CVBBDPRE Optional outputs

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

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

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

### 8. Problem reinitialization

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

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

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

### 9. Memory deallocation

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

### 10. User-supplied routines

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

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

This routine is to evaluate the function  $g(t, y)$  approximating  $f$  (possibly identical to  $f$ ), in terms of  $T = t$ , and the array YLOC (of length NLOC), which is the sub-vector of  $y$  local to this processor. The resulting (local) sub-vector is to be stored in the array GLOC. The arrays IPAR (of integers) and RPAR (of reals) contain user data and are the same as those passed to FCVMALLOC. IER is

an error return flag which should be set to 0 if successful, a positive value if a recoverable error occurred (in which case CVOICE will attempt to correct), or a negative value if FCVGLOCFN failed unrecoverably (in which case the integration is halted).

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

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



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

Optionally, the user can supply a routine FCVJTIMES for the evaluation of Jacobian-vector products, as described above in step 5 in §5.4.

## Chapter 6

# Description of the NVECTOR module

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

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, long int *, long int *);  
    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    (*nv11norm)(N_Vector);
void        (*nvcompare)(realtype, N_Vector, N_Vector);
boolean_t   (*nvinvtest)(N_Vector, N_Vector);
boolean_t   (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
realtype    (*nvminquotient)(N_Vector, N_Vector);
};

```

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 6.2 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 6.1. It is recommended that a user-supplied NVECTOR implementation use the `SUNDIALS_NVEC_CUSTOM` identifier.

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

Vector ID	Vector type	ID Value
SUNDIALS_NVEC_SERIAL	Serial	0
SUNDIALS_NVEC_PARALLEL	Distributed memory parallel (MPI)	1
SUNDIALS_NVEC_OPENMP	OpenMP shared memory parallel	2
SUNDIALS_NVEC_PTHREADS	PThreads shared memory parallel	3
SUNDIALS_NVEC_PARHYP	<i>hypre</i> ParHyp parallel vector	4
SUNDIALS_NVEC_PETSC	PETSc parallel vector	5
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	6

Table 6.2: Description of the NVECTOR operations

Name	Usage and Description
N_VGetVectorID	<code>id = N_VGetVectorID(w);</code> Returns the vector type identifier for the vector <code>w</code> . It is used to determine the vector implementation type (e.g. serial, parallel,...) from the abstract <code>N_Vector</code> interface. Returned values are given in Table 6.1.
N_VClone	<code>v = N_VClone(w);</code> 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> 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> 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> 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	

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Name	Usage and Description
<code>N_VGetArrayPointer</code>	<code>vdata = N_VGetArrayPointer(v);</code> Returns a pointer to a <b>realtype</b> array from the <b>N_Vector</b> <code>v</code> . 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.
<code>N_VSetArrayPointer</code>	<code>N_VSetArrayPointer(vdata, v);</code> 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.
<code>N_VLinearSum</code>	<code>N_VLinearSum(a, x, b, y, z);</code> Performs the operation $z = ax + by$ , where $a$ and $b$ are <b>realtype</b> scalars and $x$ and $y$ are of type <b>N_Vector</b> : $z_i = ax_i + by_i$ , $i = 0, \dots, n-1$ .
<code>N_VConst</code>	<code>N_VConst(c, z);</code> Sets all components of the <b>N_Vector</b> <code>z</code> to <b>realtype</b> <code>c</code> : $z_i = c$ , $i = 0, \dots, n-1$ .
<code>N_VProd</code>	<code>N_VProd(x, y, z);</code> Sets the <b>N_Vector</b> <code>z</code> to be the component-wise product of the <b>N_Vector</b> inputs <code>x</code> and <code>y</code> : $z_i = x_i y_i$ , $i = 0, \dots, n-1$ .
<code>N_VDiv</code>	<code>N_VDiv(x, y, z);</code> Sets the <b>N_Vector</b> <code>z</code> to be the component-wise ratio of the <b>N_Vector</b> inputs <code>x</code> and <code>y</code> : $z_i = x_i / y_i$ , $i = 0, \dots, n-1$ . The $y_i$ may not be tested for 0 values. It should only be called with a <code>y</code> that is guaranteed to have all nonzero components.
<code>N_VScale</code>	<code>N_VScale(c, x, z);</code> Scales the <b>N_Vector</b> <code>x</code> by the <b>realtype</b> scalar <code>c</code> and returns the result in <code>z</code> : $z_i = cx_i$ , $i = 0, \dots, n-1$ .
<code>N_VAbs</code>	<code>N_VAbs(x, z);</code> Sets the components of the <b>N_Vector</b> <code>z</code> to be the absolute values of the components of the <b>N_Vector</b> <code>x</code> : $z_i =  x_i $ , $i = 0, \dots, n-1$ .
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Name	Usage and Description
N_VInv	<p><code>N_VInv(x, z);</code>  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>  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>  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>  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>  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>  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>:  <math>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>  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>  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>  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>  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>
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Name	Usage and Description
N_VInvTest	<pre>t = N_VInvTest(x, z);</pre> <p>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: <math>z_i = 1.0/x_i</math>, <math>i = 0, \dots, n-1</math>. This routine returns a boolean assigned to <code>TRUE</code> if all components of <code>x</code> are nonzero (successful inversion) and returns <code>FALSE</code> otherwise.</p>
N_VConstrMask	<pre>t = N_VConstrMask(c, x, m);</pre> <p>Performs the following constraint tests: <math>x_i &gt; 0</math> if <math>c_i = 2</math>, <math>x_i \geq 0</math> if <math>c_i = 1</math>, <math>x_i \leq 0</math> if <math>c_i = -1</math>, <math>x_i &lt; 0</math> if <math>c_i = -2</math>. There is no constraint on <math>x_i</math> if <math>c_i = 0</math>. This routine returns a boolean assigned to <code>FALSE</code> if any element failed the constraint test and assigned to <code>TRUE</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.</p>
N_VMinQuotient	<pre>minq = N_VMinQuotient(num, denom);</pre> <p>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.</p>

## 6.1 The NVECTOR\_SERIAL implementation

The serial implementation of the NVECTOR module provided with SUNDIALS, `NVECTOR_SERIAL`, defines the *content* field of `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, and a boolean flag *own\_data* which specifies the ownership of *data*.

```
struct _N_VectorContent_Serial {
    long int length;
    booleantype own_data;
    realtype *data;
};
```

The header file to be included when using this module is `nvector_serial.h`.

The following five 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 6.2. Their names are obtained from those in Table 6.2 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(long int vec_length);
```

- **N\_VNewEmpty\_Serial**

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

```
N_Vector N_VNewEmpty_Serial(long int 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(long int 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.

```
long int 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);
```

## 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 = FALSE`. `N_VDestroy_Serial` and `N_VDestroyVectorArray_Serial` will not attempt to free the pointer `data` for any `N_Vector` with `own_data` set to `FALSE`. In such a case, it is the user's responsibility to deallocate the `data` pointer.



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

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

## 6.2 The NVECTOR\_PARALLEL implementation

The `NVECTOR_PARALLEL` implementation of the `NVECTOR` module provided with `SUNDIALS` is based on `MPI`. It defines the `content` field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the beginning of a contiguous local data array, an `MPI` communicator, and a boolean flag `own_data` indicating ownership of the data array `data`.

```
struct _N_VectorContent_Parallel {
    long int local_length;
    long int global_length;
    boolean_t own_data;
    realtype *data;
    MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_parallel.h`.

The following seven macros are provided to access the content of a `NVECTOR_PARALLEL` vector. The suffix `_P` in the names denotes the distributed memory parallel version.

- `NV_CONTENT_P`

This macro gives access to the contents of the parallel vector `N_Vector`.

The assignment `v_cont = NV_CONTENT_P(v)` sets `v_cont` to be a pointer to the `N_Vector` content structure of type `struct _N_VectorContent_Parallel`.

Implementation:

```
#define NV_CONTENT_P(v) ( (_N_VectorContent_Parallel)(v->content) )
```



- `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,
                          long int local_length,
                          long int 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).

```
long int N_VGetLength_Parallel(N_Vector v);
```

- `N_VGetLocalLength_Parallel`

This function returns the local vector length.

```
long int N_VGetLocalLength_Parallel(N_Vector v);
```

- `N_VPrint_Parallel`

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

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

## 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 = FALSE`. `N_VDestroy_Parallel` and `N_VDestroyVectorArray_Parallel` will not attempt to free the pointer `data` for any `N_Vector` with `own_data` set to `FALSE`. In such a case, it is the user's responsibility to deallocate the `data` pointer.



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

For solvers that include a Fortran interface module, the NVECTOR\_PARALLEL module also includes a Fortran-callable function FNVINITP(COMM, code, NLOCAL, NGLOBAL, IER), to initialize this NVECTOR\_PARALLEL module. Here COMM is the MPI communicator, code is an input solver id (1 for CVODE, 2 for IDA, 3 for KINSOL, 4 for ARKODE); NLOCAL and NGLOBAL are the local and global vector sizes, respectively (declared so as to match C type long int); and IER is an error return flag equal 0 for success and -1 for failure. NOTE: If the header file sundials\_config.h defines SUNDIALS\_MPI\_COMM\_F2C to be 1 (meaning the MPI implementation used to build SUNDIALS includes the MPI\_Comm\_f2c function), then COMM can be any valid MPI communicator. Otherwise, MPI\_COMM\_WORLD will be used, so just pass an integer value as a placeholder.



## 6.3 The NVECTOR\_OPENMP implementation

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

The OpenMP NVECTOR implementation provided with SUNDIALS, NVECTOR\_OPENMP, defines the *content* field of *N\_Vector* to be a structure containing the length of the vector, a pointer to the beginning of a contiguous data array, a boolean flag *own\_data* which specifies the ownership of *data*, and the number of threads. Operations on the vector are threaded using OpenMP.

```
struct _N_VectorContent_OpenMP {
    long int length;
    booleantype own_data;
    realtype *data;
    int num_threads;
};
```

The header file to be included when using this module is `nvector_openmp.h`.

The following six 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 6.2. Their names are obtained from those in Table 6.2 by appending the suffix `_OpenMP` (e.g. `NV_Destroy_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(long int 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(long int 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(long int 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.

```
long int N_VGetLength_OpenMP(N_Vector v);
```

- N\_VPrint\_OpenMP

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

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

## 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 = FALSE`. `N_VDestroy_OpenMP` and `N_VDestroyVectorArray_OpenMP` will not attempt to free the pointer `data` for any `N_Vector` with `own_data` set to `FALSE`. 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 `NVECTOR_OPENMP` module. Here `code` is an input solver id (1 for `CVODE`, 2 for `IDA`, 3 for `KINSOL`, 4 for `ARKODE`); `NEQ` is the problem size (declared so as to match C type `long int`); `NUMTHREADS` is the number of threads; and `IER` is an error return flag equal 0 for success and -1 for failure.

## 6.4 The NVECTOR\_PTHREADS implementation

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

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

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

The header file to be included when using this module is `nvector_pthreads.h`.

The following six 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 6.2. Their names are obtained from those in Table 6.2 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(long int 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(long int 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(long int 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.

```
long int 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);
```

### 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 = FALSE`. `N_VDestroy_Pthreads` and `N_VDestroyVectorArray_Pthreads` will not attempt to free the pointer `data` for any `N_Vector` with `own_data` set to `FALSE`. In such a case, it is the user's responsibility to deallocate the `data` pointer.
- To maximize efficiency, vector operations in the `NVECTOR_PTHREADS` implementation that have more than one `N_Vector` argument do not check for consistent internal representation of these vectors. It is the user's responsibility to ensure that such routines are called with `N_Vector` arguments that were all created with the same internal representations.



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

## 6.5 The NVECTOR\_PARHYP implementation

The `NVECTOR_PARHYP` implementation of the `NVECTOR` module provided with `SUNDIALS` is a wrapper around `hypre`'s `ParVector` class. Most of the vector kernels simply call `hypre` vector operations. The implementation defines the `content` field of `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to an object of type `hypre_ParVector`, an MPI communicator, and a boolean flag `own_parvector` indicating ownership of the `hypre` parallel vector object `x`.

```
struct _N_VectorContent_ParHyp {
    long int local_length;
    long int global_length;
    boolean_t own_parvector;
    MPI_Comm comm;
    hypre_ParVector *x;
};
```

The header file to be included when using this module is `nvector_parhyp.h`. Unlike native `SUNDIALS` vector types, `NVECTOR_PARHYP` does not provide macros to access its member variables.

The `NVECTOR_PARHYP` module defines implementations of all vector operations listed in Table 6.2, except for `N_VSetArrayPointer` and `N_VGetArrayPointer`, because accessing raw vector data is

handled by low-level *hypr* 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 *hypr* vector first, and then use *hypr* methods to access the data. Usage examples of NVECTOR\_PARHYP are provided in the `cvAdvDiff_non_ph.c` example program for CVODE [19] and the `ark_diurnal_kry_ph.c` example program for ARKODE [25].

The names of parhyp methods are obtained from those in Table 6.2 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* vector set to `NULL`.

```
N_Vector N_VNewEmpty_ParHyp(MPI_Comm comm,
                             long int local_length,
                             long int global_length);
```

- `N_VMake_ParHyp`

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

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

- `N_VGetVector_ParHyp`

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

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

- `N_VCloneVectorArray_ParHyp`

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

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

- `N_VCloneVectorArrayEmpty_ParHyp`

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

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

- `N_VDestroyVectorArray_ParHyp`

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

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

- `N_VPrint_ParHyp`

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

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

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

## 6.6 The NVECTOR\_PETSC implementation

The `NVECTOR_PETSC` module is an `NVECTOR` wrapper around the PETSc vector. It defines the *content* field of a `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the PETSc vector, an MPI communicator, and a boolean flag *own\_data* indicating ownership of the wrapped PETSc vector.

```
struct _N_VectorContent_Petsc {
    long int local_length;
    long int global_length;
    boolean_t own_data;
    Vec *pvec;
    MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_petsc.h`. 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 6.2, 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 [20].

The names of vector operations are obtained from those in Table 6.2 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,
                           long int local_length,
                           long int 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 content of a wrapped PETSc vector to stdout.

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

## 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 `FALSE`. `N_VDestroy_Petsc` and `N_VDestroyVectorArray_Petsc` will not attempt to free the pointer `pvec` for any `N_Vector` with `own_data` set to `FALSE`. In such a case, it is the user's responsibility to deallocate the `pvec` pointer.



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

## 6.7 NVECTOR Examples

There are `NVector` examples that may be installed for each implementation: serial, parallel, OpenMP, and Pthreads. 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.

## 6.8 NVECTOR functions used by CVODE

In Table 6.3 below, we list the vector functions in the NVECTOR module used within the CVODE package. The table also shows, for each function, which of the code modules uses the function. The CVODE column shows function usage within the main integrator module, while the remaining seven columns show function usage within each of the eight CVODE linear solvers, the CVBANDPRE and CVBBDPRE preconditioner modules, and the FCVODE module. Here CVDLS stands for CVDENSE and CVBAND; CVSPILS stands for CVSPGMR, CVSPBCG, and CVSPTFQMR; and CVSLS stands for CVKLU and CVSUPERLUMT.

There is one subtlety in the CVSPILS column hidden by the table, explained here for the case of the CVSPGMR module. The `N_VDotProd` function is called both within the interface file `cvode_spgmr.c` and within the implementation files `sundials_spgmr.c` and `sundials_iterative.c` for the generic SPGMR solver upon which the CVSPGMR solver is built. Also, although `N_VDiv` and `N_VProd` are not called within the interface file `cvode_spgmr.c`, they are called within the implementation file `sundials_spgmr.c`, and so are required by the CVSPGMR solver module. Analogous statements apply to the CVSPBCG and CVSPTFQMR modules, except that they do not use `sundials_iterative.c`. This issue does not arise for the other three CVODE linear solvers because the generic DENSE and BAND solvers (used in the implementation of CVDENSE and CVBAND) do not make calls to any vector functions and CVDIAG is not implemented using a generic diagonal solver.

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

The vector functions listed in Table 6.2 that are *not* used by CVODE are: `N_VWL2Norm`, `N_VL1Norm`, `N_VWrmsNormMask`, `N_VConstrMask`, and `N_VMinQuotient`. Therefore a user-supplied NVECTOR module for CVODE could omit these five functions.

Table 6.3: List of vector functions usage by CVOICE code modules

	CVOICE	CVDLS	CVDIAG	CVSPILS	CVSLS	CVBANDPRE	CVBDDPRE	FCVOICE
N_VGetVectorID								
N_VClone	✓		✓	✓				
N_VCloneEmpty								✓
N_VDestroy	✓		✓	✓				
N_VSpace	✓							
N_VGetArrayPointer		✓			✓	✓	✓	✓
N_VSetArrayPointer		✓						✓
N_VLinearSum	✓	✓	✓	✓				
N_VConst	✓			✓				
N_VProd	✓		✓	✓				
N_VDiv	✓		✓	✓				
N_VScale	✓	✓	✓	✓	✓	✓	✓	
N_VAbs	✓							
N_VInv	✓		✓					
N_VAddConst	✓		✓					
N_VDotProd				✓				
N_VMaxNorm	✓							
N_VWrmsNorm	✓	✓		✓		✓	✓	
N_VMin	✓							
N_VCompare			✓					
N_VInvTest			✓					



## Chapter 7

# Providing Alternate Linear Solver Modules

The central CVODE module interfaces with a linear solver module by way of calls to four functions. These are denoted here by `linit`, `lsetup`, `lsolve`, and `lfree`. Briefly, their purposes are as follows:

- `linit`: initialize memory specific to the linear solver;
- `lsetup`: evaluate and preprocess the Jacobian or preconditioner;
- `lsolve`: solve the linear system;
- `lfree`: free the linear solver memory.

A linear solver module must also provide a user-callable **specification function** (like those described in §4.5.3) which will attach the above four functions to the main CVODE memory block. The CVODE memory block is a structure defined in the header file `cvode_impl.h`. A pointer to such a structure is defined as the type `CVodeMem`. The four fields in a `CVodeMem` structure that must point to the linear solver's functions are `cv_linit`, `cv_lsetup`, `cv_lsolve`, and `cv_lfree`, respectively. Note that of the four interface functions, only the `lsolve` function is required. The `lfree` function must be provided only if the solver specification function makes any memory allocation. For any of the functions that are *not* provided, the corresponding field should be set to `NULL`. The linear solver specification function must also set the value of the field `cv_setupNonNull` in the CVODE memory block — to `TRUE` if `lsetup` is used, or `FALSE` otherwise.

Typically, the linear solver will require a block of memory specific to the solver, and a principal function of the specification function is to allocate that memory block, and initialize it. Then the field `cv_lmem` in the CVODE memory block is available to attach a pointer to that linear solver memory. This block can then be used to facilitate the exchange of data between the four interface functions.

If the linear solver involves adjustable parameters, the specification function should set the default values of those. User-callable functions may be defined that could, optionally, override the default parameter values.

We encourage the use of performance counters in connection with the various operations involved with the linear solver. Such counters would be members of the linear solver memory block, would be initialized in the `linit` function, and would be incremented by the `lsetup` and `lsolve` functions. Then, user-callable functions would be needed to obtain the values of these counters.

For consistency with the existing CVODE linear solver modules, we recommend that the return value of the specification function be 0 for a successful return, and a negative value if an error occurs. Possible error conditions include: the pointer to the main CVODE memory block is `NULL`, an input is illegal, the `NVECTOR` implementation is not compatible, or a memory allocation fails.

These four functions, which interface between CVODE and the linear solver module, necessarily have fixed call sequences. Thus, a user wishing to implement another linear solver within the CVODE

package must adhere to this set of interfaces. The following is a complete description of the call list for each of these functions. Note that the call list of each function includes a pointer to the main CVODE memory block, by which the function can access various data related to the CVODE solution. The contents of this memory block are given in the file `cvode_impl.h` (but not reproduced here, for the sake of space).

## 7.1 Initialization function

The type definition of `linit` is

`linit`

Definition `int (*linit)(CNodeMem cv_mem);`

Purpose The purpose of `linit` is to complete initializations for the specific linear solver, such as counters and statistics. It should also set pointers to data blocks that will later be passed to functions associated with the linear solver. The `linit` function is called once only, at the start of the problem, during the first call to `CNode`.

Arguments `cv_mem` is the CVODE memory pointer of type `CNodeMem`.

Return value An `linit` function should return 0 if it has successfully initialized the CVODE linear solver, and a negative value otherwise.

## 7.2 Setup function

The type definition of `lsetup` is

`lsetup`

Definition `int (*lsetup)(CNodeMem cv_mem, int convfail, N_Vector ypred,  
N_Vector fpred, booleantype *jcurPtr,  
N_Vector vtemp1, N_Vector vtemp2, N_Vector vtemp3);`

Purpose The job of `lsetup` is to prepare the linear solver for subsequent calls to `lsolve`, in the solution of systems  $Mx = b$ , where  $M$  is some approximation to the Newton matrix,  $I - \gamma \partial f / \partial y$ . (See Eq.(2.5)). Here  $\gamma$  is available as `cv_mem->cv_gamma`.

The `lsetup` function may call a user-supplied function, or a function within the linear solver module, to compute needed data related to the Jacobian matrix  $\partial f / \partial y$ . Alternatively, it may choose to retrieve and use stored values of this data.

In either case, `lsetup` may also preprocess that data as needed for `lsolve`, which may involve calling a generic function (such as for LU factorization). This data may be intended either for direct use (in a direct linear solver) or for use in a preconditioner (in a preconditioned iterative linear solver).

The `lsetup` function is not called at every time step, but only as frequently as the solver determines that it is appropriate to perform the setup task. In this way, Jacobian-related data generated by `lsetup` is expected to be used over a number of time steps.

Arguments `cv_mem` is the CVODE memory pointer of type `CNodeMem`.

`convfail` is an input flag used to indicate any problem that occurred during the solution of the nonlinear equation on the current time step for which the linear solver is being used. This flag can be used to help decide whether the Jacobian data kept by a CVODE linear solver needs to be updated or not. Its possible values are:

- **CV\_NO\_FAILURES**: this value is passed to **lsetup** if either this is the first call for this step, or the local error test failed on the previous attempt at this step (but the Newton iteration converged).
- **CV\_FAIL\_BAD\_J**: this value is passed to **lsetup** if (a) the previous Newton corrector iteration did not converge and the linear solver's setup function indicated that its Jacobian-related data is not current, or (b) during the previous Newton corrector iteration, the linear solver's solve function failed in a recoverable manner and the linear solver's setup function indicated that its Jacobian-related data is not current.
- **CV\_FAIL\_OTHER**: this value is passed to **lsetup** if during the current internal step try, the previous Newton iteration failed to converge even though the linear solver was using current Jacobian-related data.

**ypred** is the predicted **y** vector for the current CVODE internal step.  
**fpred** is the value of the right-hand side at **ypred**,  $f(t_n, \text{ypred})$ .  
**jcurPtr** is a pointer to a boolean to be filled in by **lsetup**. The function should set **\*jcurPtr** = **TRUE** if its Jacobian data is current after the call, and should set **\*jcurPtr** = **FALSE** if its Jacobian data is not current. If **lsetup** calls for re-evaluation of Jacobian data (based on **convfail** and CVODE state data), it should return **\*jcurPtr** = **TRUE** unconditionally; otherwise an infinite loop can result.  
**vtemp1**  
**vtemp2**  
**vtemp3** are temporary variables of type **N.Vector** provided for use by **lsetup**.

**Return value** The **lsetup** function should return 0 if successful, a positive value for a recoverable error, and a negative value for an unrecoverable error. On a recoverable error return, the solver will attempt to recover by reducing the step size.

## 7.3 Solve function

The type definition of **lsolve** is

**lsolve**

**Definition** `int (*lsolve)(CvodeMem cv_mem, N_Vector b, N_Vector weight,  
N_Vector ycur, N_Vector fcur);`

**Purpose** The function **lsolve** must solve the linear system  $Mx = b$ , where  $M$  is some approximation to the Newton matrix,  $I - \gamma J$ , where  $J = (\partial f / \partial y)(t_n, y_{cur})$  (see Eq.(2.5)), and the right-hand side vector,  $b$ , is input. Here  $\gamma$  is available as **cv\_mem->cv\_gamma**.

**lsolve** is called once per Newton iteration, hence possibly several times per time step.

If there is an **lsetup** function, this **lsolve** function should make use of any Jacobian data that was computed and preprocessed by **lsetup**, either for direct use, or for use in a preconditioner.

**Arguments** **cv\_mem** is the CVODE memory pointer of type **CvodeMem**.

**b** is the right-hand side vector  $b$ . The solution is to be returned in the vector **b**.

**weight** is a vector that contains the error weights. These are the  $W_i$  of Eq.(2.6). This weight vector is included here to enable the computation of weighted norms needed to test for the convergence of iterative methods (if any) within the linear solver.

**ycur** is a vector that contains the solver's current approximation to  $y(t_n)$ .

**fcur** is a vector that contains the current right-hand side,  $f(t_n, ycur)$ .

**Return value** The `lsolve` function should return a positive value for a recoverable error and a negative value for an unrecoverable error. Success is indicated by a 0 return value. On a recoverable error return, the solver will attempt to recover, such as by calling the `lsetup` function with current arguments.

## 7.4 Memory deallocation function

The type definition of `lfree` is

`lfree`

**Definition**     `int (*lfree)(CNodeMem cv_mem);`

**Purpose**         The function `lfree` should free up any memory allocated by the linear solver.

**Arguments**     The argument `cv_mem` is the `CVODE` memory pointer of type `CNodeMem`.

**Return value**   The `lfree` function should return 0 if successful, or a nonzero if not.

**Notes**          This function is called once a problem has been completed and the linear solver is no longer needed.

## Chapter 8

# General Use Linear Solver Components in SUNDIALS

In this chapter, we describe linear solver code components that are included in SUNDIALS, but which are of potential use as generic packages in themselves, either in conjunction with the use of SUNDIALS or separately.

These generic modules in SUNDIALS are organized in three families, the *dls* family, which includes direct linear solvers appropriate for sequential computations; the *sls* family, which includes sparse matrix solvers; and the *spils* family, which includes scaled preconditioned iterative (Krylov) linear solvers. The solvers in each family share common data structures and functions.

The *dls* family contains the following two generic linear solvers:

- The DENSE package, a linear solver for dense matrices either specified through a matrix type (defined below) or as simple arrays.
- The BAND package, a linear solver for banded matrices either specified through a matrix type (defined below) or as simple arrays.

Note that this family also includes the Blas/Lapack linear solvers (dense and band) available to the SUNDIALS solvers, but these are not discussed here.

The *sls* family contains a sparse matrix package and interfaces between it and two sparse direct solver packages:

- The KLU package, a linear solver for compressed-sparse-column matrices, [1, 11].
- The SUPERLUMT package, a threaded linear solver for compressed-sparse-column matrices, [2, 23, 12].

The *spils* family contains the following generic linear solvers:

- The SPGMR package, a solver for the scaled preconditioned GMRES method.
- The SPFGMR package, a solver for the scaled preconditioned Flexible GMRES method.
- The SPBCG package, a solver for the scaled preconditioned Bi-CGStab method.
- The SPTFQMR package, a solver for the scaled preconditioned TFQMR method.

For reasons related to installation, the names of the files involved in these packages begin with the prefix `sundials_`. But despite this, each of the *dls* and *spils* solvers is in fact generic, in that it is usable completely independently of SUNDIALS.

For the sake of space, the functions for the `dense` and `band` modules that work with a matrix type, and the functions in the SPGMR, SPFGMR, SPBCG, and SPTFQMR modules are only summarized briefly, since they are less likely to be of direct use in connection with a SUNDIALS solver. However, the

functions for dense matrices treated as simple arrays and sparse matrices are fully described, because we expect that they will be useful in the implementation of preconditioners used with the combination of one of the SUNDIALS solvers and one of the *spils* linear solvers.

## 8.1 The DLS modules: DENSE and BAND

The files comprising the DENSE generic linear solver, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir/include/sundials*)  
`sundials_direct.h`, `sundials_dense.h`,  
`sundials_types.h`, `sundials_math.h`, `sundials_config.h`
- source files (located in *srcdir/src/sundials*)  
`sundials_direct.c`, `sundials_dense.c`, `sundials_math.c`

The files comprising the BAND generic linear solver are as follows:

- header files (located in *srcdir/include/sundials*)  
`sundials_direct.h`, `sundials_band.h`,  
`sundials_types.h`, `sundials_math.h`, `sundials_config.h`
- source files (located in *srcdir/src/sundials*)  
`sundials_direct.c`, `sundials_band.c`, `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are relevant to the DENSE and BAND packages by themselves.

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:  
`#define SUNDIALS_DOUBLE_PRECISION 1`  
`#define SUNDIALS_SINGLE_PRECISION 1`  
`#define SUNDIALS_EXTENDED_PRECISION 1`
- (optional) use of generic math functions: `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the macros `SUNMIN` and `SUNMAX`, and the function `SUNRabs`.

The files listed above for either module can be extracted from the SUNDIALS *srcdir* and compiled by themselves into a separate library or into a larger user code.

### 8.1.1 Type `DlsMat`

The type `DlsMat`, defined in `sundials_direct.h` is a pointer to a structure defining a generic matrix, and is used with all linear solvers in the *dls* family:

```
typedef struct _DlsMat {
    int type;
    long int M;
    long int N;
    long int ldim;
    long int mu;
    long int ml;
    long int s_mu;
    realtype *data;
    long int ldata;
    realtype **cols;
} *DlsMat;
```

For the DENSE module, the relevant fields of this structure are as follows. Note that a dense matrix of type `DlsMat` need not be square.

**type** - `SUNDIALS_DENSE` (=1)

**M** - number of rows

**N** - number of columns

**ldim** - leading dimension ( $\text{ldim} \geq M$ )

**data** - pointer to a contiguous block of `realtype` variables

**ldata** - length of the data array ( $= \text{ldim} \cdot N$ ). The  $(i,j)$ -th element of a dense matrix **A** of type `DlsMat` (with  $0 \leq i < M$  and  $0 \leq j < N$ ) is given by the expression `(A->data)[0][j*M+i]`

**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 matrix **A** of type `DlsMat` (with  $0 \leq i < M$  and  $0 \leq j < N$ ) is given by the expression `(A->cols)[j][i]`

For the BAND module, the relevant fields of this structure are as follows (see Figure 8.1 for a diagram of the underlying data representation in a banded matrix of type `DlsMat`). Note that only square band matrices are allowed.

**type** - `SUNDIALS_BAND` (=2)

**M** - number of rows

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

**mu** - upper half-bandwidth,  $0 \leq \text{mu} < \min(M,N)$

**ml** - lower half-bandwidth,  $0 \leq \text{ml} < \min(M,N)$

**s\_mu** - storage upper bandwidth,  $\text{mu} \leq \text{s\_mu} < N$ . The LU decomposition routine writes the LU factors into the storage for **A**. The upper triangular factor **U**, however, may have an upper bandwidth as big as  $\min(N-1, \text{mu}+\text{ml})$  because of partial pivoting. The **s\_mu** field holds the upper half-bandwidth allocated for **A**.

**ldim** - leading dimension ( $\text{ldim} \geq \text{s\_mu}$ )

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

**ldata** - length of the data array ( $= \text{ldim} \cdot (\text{s\_mu} + \text{ml} + 1)$ )

**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  $\text{s\_mu}-\text{mu}$  (to access the uppermost element within the band in the  $j$ -th column) to  $\text{s\_mu}+\text{ml}$  (to access the lowest element within the band in the  $j$ -th column). Indices from 0 to  $\text{s\_mu}-\text{mu}-1$  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,  $j-\text{mu} \leq i \leq j+\text{ml}$ .

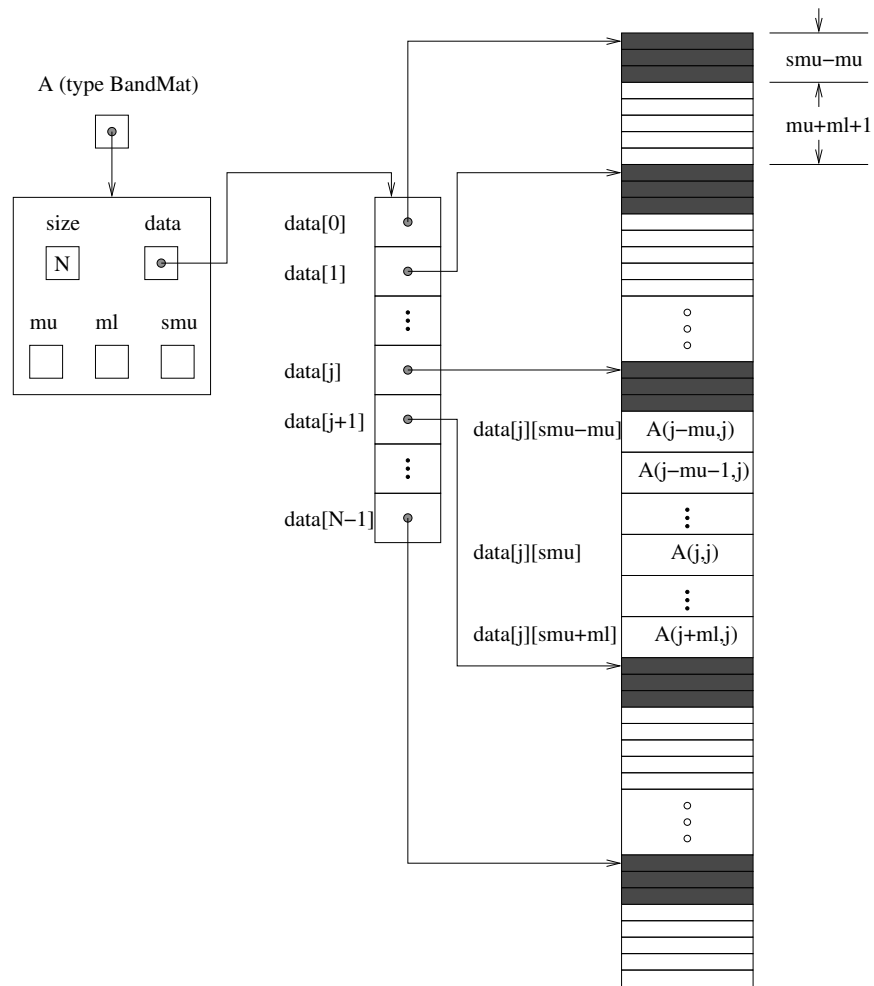


Figure 8.1: Diagram of the storage for a banded matrix of type `DlsMat`. Here  $A$  is an  $N \times N$  band matrix of type `DlsMat` with upper and lower half-bandwidths `mu` and `ml`, respectively. The rows and columns of  $A$  are numbered from 0 to  $N - 1$  and the  $(i, j)$ -th element of  $A$  is denoted  $A(i, j)$ . The greyed out areas of the underlying component storage are used by the `BandGBTRF` and `BandGBTRS` routines.

### 8.1.2 Accessor macros for the DLS modules

The macros below allow a user to efficiently access individual matrix elements without writing out explicit data structure references and without knowing too much about the underlying element storage. The only storage assumption needed is that elements are stored columnwise and that a pointer to the  $j$ -th column of elements can be obtained via the `DENSE_COL` or `BAND_COL` macros. Users should use these macros whenever possible.

The following two macros are defined by the `DENSE` module to provide access to data in the `DlsMat` type:

- `DENSE_ELEM`

Usage : `DENSE_ELEM(A,i,j) = a_ij`; or `a_ij = DENSE_ELEM(A,i,j)`;

`DENSE_ELEM` references the  $(i,j)$ -th element of the  $M \times N$  `DlsMat` `A`,  $0 \leq i < M$ ,  $0 \leq j < N$ .

- `DENSE_COL`

Usage : `col_j = DENSE_COL(A,j)`;

`DENSE_COL` references the  $j$ -th column of the  $M \times N$  `DlsMat` `A`,  $0 \leq j < N$ . The type of the expression `DENSE_COL(A,j)` is `realtype *`. After the assignment in the usage above, `col_j` may be treated as an array indexed from 0 to  $M - 1$ . The  $(i, j)$ -th element of `A` is referenced by `col_j[i]`.

The following three macros are defined by the `BAND` module to provide access to data in the `DlsMat` type:

- `BAND_ELEM`

Usage : `BAND_ELEM(A,i,j) = a_ij`; or `a_ij = BAND_ELEM(A,i,j)`;

`BAND_ELEM` references 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  $j - (A \rightarrow \text{mu}) \leq i \leq j + (A \rightarrow \text{ml})$ .

- `BAND_COL`

Usage : `col_j = BAND_COL(A,j)`;

`BAND_COL` references 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 `BAND_COL(A,j)` is `realtype *`. The pointer returned by the call `BAND_COL(A,j)` can be treated as an array which is indexed from  $-(A \rightarrow \text{mu})$  to  $(A \rightarrow \text{ml})$ .

- `BAND_COL_ELEM`

Usage : `BAND_COL_ELEM(col_j,i,j) = a_ij`; or `a_ij = BAND_COL_ELEM(col_j,i,j)`;

This macro references the  $(i,j)$ -th entry of the band matrix `A` when used in conjunction with `BAND_COL` to reference the  $j$ -th column through `col_j`. The index  $(i,j)$  should satisfy  $j - (A \rightarrow \text{mu}) \leq i \leq j + (A \rightarrow \text{ml})$ .

### 8.1.3 Functions in the DENSE module

The `DENSE` module defines two sets of functions with corresponding names. The first set contains functions (with names starting with a capital letter) that act on dense matrices of type `DlsMat`. The second set contains functions (with names starting with a lower case letter) that act on matrices represented as simple arrays.

The following functions for `DlsMat` dense matrices are available in the `DENSE` package. For full details, see the header files `sundials_direct.h` and `sundials_dense.h`.

- `NewDenseMat`: allocation of a `DlsMat` dense matrix;
- `DestroyMat`: free memory for a `DlsMat` matrix;

- **PrintMat**: print a **DlsMat** matrix to standard output.
- **NewLintArray**: allocation of an array of **long int** integers for use as pivots with **DenseGETRF** and **DenseGETRS**;
- **NewIntArray**: allocation of an array of **int** integers for use as pivots with the Lapack dense solvers;
- **NewRealArray**: allocation of an array of **realtype** for use as right-hand side with **DenseGETRS**;
- **DestroyArray**: free memory for an array;
- **SetToZero**: load a matrix with zeros;
- **AddIdentity**: increment a square matrix by the identity matrix;
- **DenseCopy**: copy one matrix to another;
- **DenseScale**: scale a matrix by a scalar;
- **DenseGETRF**: LU factorization with partial pivoting;
- **DenseGETRS**: solution of  $Ax = b$  using LU factorization (for square matrices  $A$ );
- **DensePOTRF**: Cholesky factorization of a real symmetric positive matrix;
- **DensePOTRS**: solution of  $Ax = b$  using the Cholesky factorization of  $A$ ;
- **DenseGEQRF**: QR factorization of an  $m \times n$  matrix, with  $m \geq n$ ;
- **DenseORMQR**: compute the product  $w = Qv$ , with  $Q$  calculated using **DenseGEQRF**;
- **DenseMatvec**: compute the product  $y = Ax$ , for an  $M$  by  $N$  matrix  $A$ ;

The following functions for small dense matrices are available in the **DENSE** package:

- **newDenseMat**  
**newDenseMat(m,n)** allocates storage for an  $m$  by  $n$  dense matrix. It returns a pointer to the newly allocated storage if successful. If the memory request cannot be satisfied, then **newDenseMat** returns **NULL**. The underlying type of the dense matrix returned is **realtype\*\***. If we allocate a dense matrix **realtype\*\* a** by **a = newDenseMat(m,n)**, then **a[j][i]** references the  $(i,j)$ -th element of the matrix **a**,  $0 \leq i < m$ ,  $0 \leq j < n$ , and **a[j]** is a pointer to the first element in the  $j$ -th column of **a**. The location **a[0]** contains a pointer to  $m \times n$  contiguous locations which contain the elements of **a**.
- **destroyMat**  
**destroyMat(a)** frees the dense matrix **a** allocated by **newDenseMat**;
- **newLintArray**  
**newLintArray(n)** allocates an array of  $n$  integers, all **long int**. It returns a pointer to the first element in the array if successful. It returns **NULL** if the memory request could not be satisfied.
- **newIntArray**  
**newIntArray(n)** allocates an array of  $n$  integers, all **int**. It returns a pointer to the first element in the array if successful. It returns **NULL** if the memory request could not be satisfied.
- **newRealArray**  
**newRealArray(n)** allocates an array of  $n$  **realtype** values. It returns a pointer to the first element in the array if successful. It returns **NULL** if the memory request could not be satisfied.

- **destroyArray**  
`destroyArray(p)` frees the array `p` allocated by `newLintArray`, `newIntArray`, or `newRealArray`;
- **denseCopy**  
`denseCopy(a,b,m,n)` copies the `m` by `n` dense matrix `a` into the `m` by `n` dense matrix `b`;
- **denseScale**  
`denseScale(c,a,m,n)` scales every element in the `m` by `n` dense matrix `a` by the scalar `c`;
- **denseAddIdentity**  
`denseAddIdentity(a,n)` increments the *square* `n` by `n` dense matrix `a` by the identity matrix  $I_n$ ;
- **denseGETRF**  
`denseGETRF(a,m,n,p)` factors the `m` by `n` dense matrix `a`, using Gaussian elimination with row pivoting. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.  
A successful LU factorization leaves the matrix `a` and the pivot array `p` with the following information:
  1. `p[k]` contains the row number of the pivot element chosen at the beginning of elimination step `k`,  $k = 0, 1, \dots, n-1$ .
  2. If the unique LU factorization of `a` is given by  $Pa = LU$ , where  $P$  is a permutation matrix,  $L$  is an `m` by `n` lower trapezoidal matrix with all diagonal elements equal to 1, and  $U$  is an `n` by `n` upper triangular matrix, then the upper triangular part of `a` (including its diagonal) contains  $U$  and the strictly lower trapezoidal part of `a` contains the multipliers,  $I - L$ . If `a` is square,  $L$  is a unit lower triangular matrix.`denseGETRF` returns 0 if successful. Otherwise it encountered a zero diagonal element during the factorization, indicating that the matrix `a` does not have full column rank. In this case it returns the column index (numbered from one) at which it encountered the zero.
- **denseGETRS**  
`denseGETRS(a,n,p,b)` solves the `n` by `n` linear system  $ax = b$ . It assumes that `a` (of size  $n \times n$ ) has been LU-factored and the pivot array `p` has been set by a successful call to `denseGETRF(a,n,n,p)`. The solution  $x$  is written into the `b` array.
- **densePOTRF**  
`densePOTRF(a,m)` calculates the Cholesky decomposition of the `m` by `m` dense matrix `a`, assumed to be symmetric positive definite. Only the lower triangle of `a` is accessed and overwritten with the Cholesky factor.
- **densePOTRS**  
`densePOTRS(a,m,b)` solves the `m` by `m` linear system  $ax = b$ . It assumes that the Cholesky factorization of `a` has been calculated in the lower triangular part of `a` by a successful call to `densePOTRF(a,m)`.
- **denseGEQRF**  
`denseGEQRF(a,m,n,beta,wrk)` calculates the QR decomposition of the `m` by `n` matrix `a` ( $m \geq n$ ) using Householder reflections. On exit, the elements on and above the diagonal of `a` contain the `n` by `n` upper triangular matrix  $R$ ; the elements below the diagonal, with the array `beta`, represent the orthogonal matrix  $Q$  as a product of elementary reflectors. The real array `wrk`, of length `m`, must be provided as temporary workspace.

- **denseORMQR**

**denseORMQR(a,m,n,beta,v,w,wrk)** calculates the product  $w = Qv$  for a given vector **v** of length **n**, where the orthogonal matrix  $Q$  is encoded in the **m** by **n** matrix **a** and the vector **beta** of length **n**, after a successful call to **denseGEQRF(a,m,n,beta,wrk)**. The real array **wrk**, of length **m**, must be provided as temporary workspace.

- **denseMatvec**

**denseMatvec(a,x,y,m,n)** calculates the product  $y = ax$  for a given vector **x** of length **n**, and **m** by **n** matrix **a**.

### 8.1.4 Functions in the BAND module

The BAND module defines two sets of functions with corresponding names. The first set contains functions (with names starting with a capital letter) that act on band matrices of type **DlsMat**. The second set contains functions (with names starting with a lower case letter) that act on matrices represented as simple arrays.

The following functions for **DlsMat** banded matrices are available in the BAND package. For full details, see the header files **sundials\_direct.h** and **sundials\_band.h**.

- **NewBandMat**: allocation of a **DlsMat** band matrix;
- **DestroyMat**: free memory for a **DlsMat** matrix;
- **PrintMat**: print a **DlsMat** matrix to standard output.
- **NewLintArray**: allocation of an array of **int** integers for use as pivots with **BandGBRF** and **BandGBRS**;
- **NewIntArray**: allocation of an array of **int** integers for use as pivots with the Lapack band solvers;
- **NewRealArray**: allocation of an array of **realtype** for use as right-hand side with **BandGBRS**;
- **DestroyArray**: free memory for an array;
- **SetToZero**: load a matrix with zeros;
- **AddIdentity**: increment a square matrix by the identity matrix;
- **BandCopy**: copy one matrix to another;
- **BandScale**: scale a matrix by a scalar;
- **BandGBTRF**: LU factorization with partial pivoting;
- **BandGBTRS**: solution of  $Ax = b$  using LU factorization;
- **BandMatvec**: compute the product  $y = Ax$ , for a square band matrix  $A$ ;

The following functions for small band matrices are available in the BAND package:

- **newBandMat**  
**newBandMat(n, smu, ml)** allocates storage for an **n** by **n** band matrix with lower half-bandwidth **ml**.
- **destroyMat**  
**destroyMat(a)** frees the band matrix **a** allocated by **newBandMat**;

- **newLintArray**  
`newLintArray(n)` allocates an array of `n` integers, all `long int`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.
- **newIntArray**  
`newIntArray(n)` allocates an array of `n` integers, all `int`. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.
- **newRealArray**  
`newRealArray(n)` allocates an array of `n` `realtype` values. It returns a pointer to the first element in the array if successful. It returns `NULL` if the memory request could not be satisfied.
- **destroyArray**  
`destroyArray(p)` frees the array `p` allocated by `newLintArray`, `newIntArray`, or `newRealArray`;
- **bandCopy**  
`bandCopy(a,b,n,a_smu, b_smu,copymu, copyml)` copies the `n` by `n` band matrix `a` into the `n` by `n` band matrix `b`;
- **bandScale**  
`bandScale(c,a,n,mu,ml,smu)` scales every element in the `n` by `n` band matrix `a` by `c`;
- **bandAddIdentity**  
`bandAddIdentity(a,n,smu)` increments the `n` by `n` band matrix `a` by the identity matrix;
- **bandGETRF**  
`bandGETRF(a,n,mu,ml,smu,p)` factors the `n` by `n` band matrix `a`, using Gaussian elimination with row pivoting. It overwrites the elements of `a` with its LU factors and keeps track of the pivot rows chosen in the pivot array `p`.
- **bandGETRS**  
`bandGETRS(a,n,smu,ml,p,b)` solves the `n` by `n` linear system  $ax = b$ . It assumes that `a` (of size  $n \times n$ ) has been LU-factored and the pivot array `p` has been set by a successful call to `bandGETRF(a,n,mu,ml,smu,p)`. The solution `x` is written into the `b` array.
- **bandMatvec**  
`bandMatvec(a,x,y,n,mu,ml,smu)` calculates the product  $y = ax$  for a given vector `x` of length `n`, and `n` by `n` band matrix `a`.

## 8.2 The SLS module

SUNDIALS provides a compressed-sparse-column matrix type and sparse matrix support functions. In addition, SUNDIALS provides interfaces to the publically available KLU and SuperLU\_MT sparse direct solver packages. The files comprising the SLS matrix module, used in the KLU and SUPERLUMT linear solver packages, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir/include/sundials*)  
`sundials_sparse.h`, `sundials_klu_impl.h`,  
`sundials_superluml_t_impl.h`, `sundials_types.h`,  
`sundials_math.h`, `sundials_config.h`
- source files (located in *srcdir/src/sundials*)  
`sundials_sparse.c`, `sundials_math.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are relevant to the SLS package by itself:

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:
 

```
#define SUNDIALS_DOUBLE_PRECISION 1
#define SUNDIALS_SINGLE_PRECISION 1
#define SUNDIALS_EXTENDED_PRECISION 1
```
- (optional) use of generic math functions: `#define SUNDIALS_USE_GENERIC_MATH 1`

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the macros `SUNMIN` and `SUNMAX`, and the function `SUNRabs`.

### 8.2.1 Type `SlsMat`

SUNDIALS supports operations with compressed-sparse-column (CSC) and compressed-sparse-row (CSR) matrices. For convenience integer sparse matrix identifiers are defined as:

```
#define CSC_MAT 0
#define CSR_MAT 1
```

The type `SlsMat`, defined in `sundials_sparse.h` is a pointer to a structure defining generic CSC and CSR matrix formats, and is used with all linear solvers in the *sls* family:

```
typedef struct _SlsMat {
    int M;
    int N;
    int NNZ;
    int NP;
    realtype *data;
    int sparsetype;
    int *indexvals;
    int *indexptrs;
    int **rowvals;
    int **colptrs;
    int **colvals;
    int **rowptrs;
} *SlsMat;
```

The fields of this structure are as follows (see Figure 8.2 for a diagram of the underlying compressed-sparse-column representation in a sparse matrix of type `SlsMat`). Note that a sparse matrix of type `SlsMat` need not be square.

**M** - number of rows

**N** - number of columns

**NNZ** - maximum number of nonzero entries in the matrix (allocated length of `data` and `rowvals` 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 by the `SparseNewMat` function, 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 a `SlsMat` 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};
rowvals = &indexvals;
colptrs = &indexptrs;
colvals = NULL;
rowptrs = NULL;
```

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. The work associated with operations on the sparse matrix is proportional to this value and so one should use the best understanding of the number of nonzeros here.

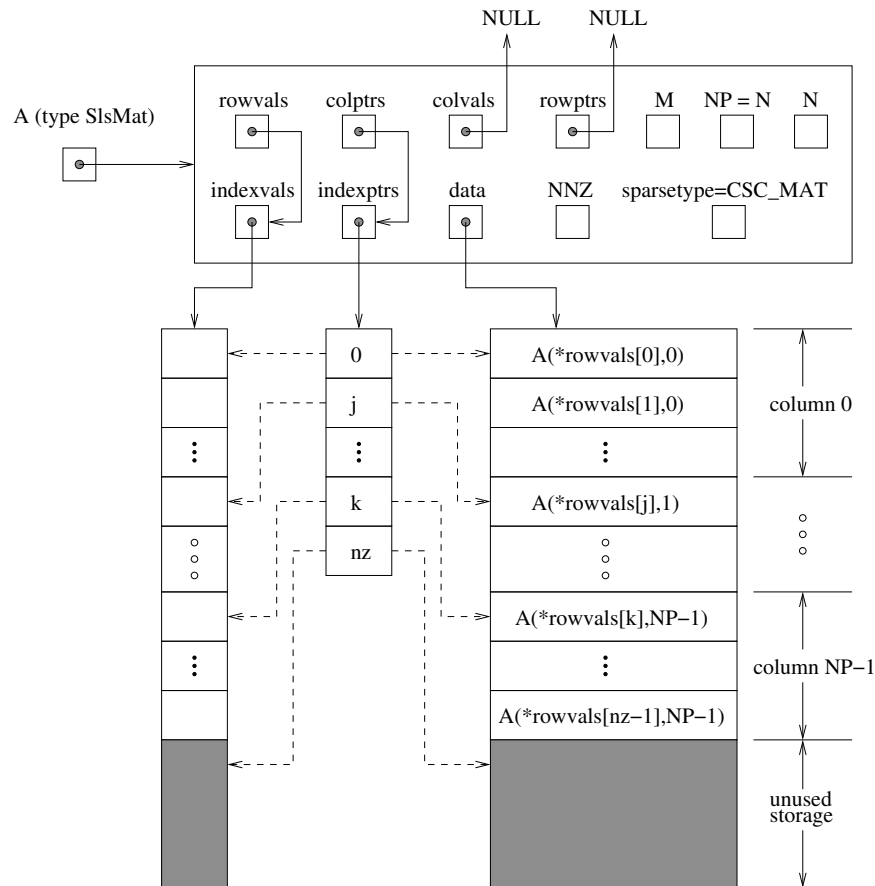


Figure 8.2: Diagram of the storage for a compressed-sparse-column matrix of type `SlsMat`. Here  $A$  is an  $M \times N$  sparse matrix of type `SlsMat` with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from 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.

### 8.2.2 Functions in the SLS module

The SLS module defines functions that act on sparse matrices of type `SlsMat`. For full details, see the header file `sundials_sparse.h`.

- **SparseNewMat**

`SparseNewMat(M, N, NNZ, sparsetype)` allocates storage for an  $M$  by  $N$  sparse matrix, with storage for up to `NNZ` nonzero entries and `sparsetype` storage type (`CSC_MAT` or `CSR_MAT`).

- **SparseFromDenseMat**

`SparseFromDenseMat(A)` converts a dense or band matrix `A` of type `DlsMat` into a new `CSC` matrix of type `SlsMat` by retaining only the nonzero values of the matrix `A`.

- **SparseDestroyMat**

`SparseDestroyMat(A)` frees the memory for a sparse matrix `A` allocated by either `SparseNewMat` or `SparseFromDenseMat`.

- **SparseSetMatToZero(A)** zeros out the `SlsMat` matrix `A`. The storage for `A` is left unchanged.

- **SparseCopyMat**

`SparseCopyMat(A, B)` copies the `SlsMat` `A` into the `SlsMat` `B`. It is assumed that the matrices have the same row/column dimensions and storage type. If `B` has insufficient storage to hold all the nonzero entries of `A`, the data and index arrays in `B` are reallocated to match those in `A`.

- **SparseScaleMat**

`SparseScaleMat(c, A)` scales every element in the `SlsMat` `A` by the `realtype` scalar `c`.

- **SparseAddIdentityMat**

`SparseAddIdentityMat(A)` increments the `SlsMat` `A` by the identity matrix. If `A` is not square, only the existing diagonal values are incremented. Resizes the `data` and `rowvals` arrays of `A` to allow for new nonzero entries on the diagonal.

- **SparseAddMat**

`SparseAddMat(A, B)` adds two `SlsMat` matrices `A` and `B`, placing the result back in `A`. Resizes the `data` and `rowvals` arrays of `A` upon completion to exactly match the nonzero storage for the result. Upon successful completion, the return value is zero; otherwise -1 is returned. It is assumed that both matrices have the same size and storage type.

- **SparseReallocMat**

`SparseReallocMat(A)` eliminates unused storage in the `SlsMat` `A` by resizing the internal `data` and `rowvals` arrays to contain exactly `colptrs[N]` values.

- **SparseMatvec**

`SparseMatvec(A, x, y)` computes the sparse matrix-vector product,  $y = Ax$ . If the `SlsMat` `A` is a sparse matrix of dimension  $M \times N$ , then it is assumed that `x` is a `realtype` array of length  $N$ , and `y` is a `realtype` array of length  $M$ . Upon successful completion, the return value is zero; otherwise -1 is returned.

- **SparsePrintMat**

`SparsePrintMat(A)` Prints the `SlsMat` matrix `A` to standard output.

### 8.2.3 The KLU solver

KLU is a sparse matrix factorization and solver library written by Tim Davis [1, 11]. KLU 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). Note that SUNDIALS uses the COLAMD ordering by default with KLU.

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.

The KLU interface in SUNDIALS will perform the symbolic factorization once. It then calls the numerical factorization once and will call the refactor routine until estimates of the numerical conditioning suggest a new factorization should be completed. The KLU interface also has a `ReInit` routine that can be used to force a full refactorization at the next solver setup call.

In order to use the SUNDIALS 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).

Designed for serial calculations only, KLU is supported for calculations employing SUNDIALS' serial or shared-memory parallel NVECTOR modules (see Sections 6.1, 6.3 and 6.4 for details).

### 8.2.4 The SUPERLUMT solver

SUPERLUMT is a threaded sparse matrix factorization and solver library written by X. Sherry Li [2, 23, 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 SUNDIALS 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).

Designed for serial and threaded calculations only, SUPERLUMT is supported for calculations employing SUNDIALS' serial or shared-memory parallel NVECTOR modules (see Sections 6.1, 6.3 and 6.4 for details).

## 8.3 The SPILS modules: SPGMR, SPFGMR, SPBCG, and SPTFQMR

The *spils* modules contain implementations of some of the most commonly use scaled preconditioned Krylov solvers. A linear solver module from the *spils* family can be used in conjunction with any NVECTOR implementation library.

### 8.3.1 The SPGMR module

The SPGMR package, in the files `sundials_spgmr.h` and `sundials_spgmr.c`, includes an implementation of the scaled preconditioned GMRES method. A separate code module, implemented in `sundials_iterative.(h,c)`, contains auxiliary functions that support SPGMR, as well as the other Krylov solvers in SUNDIALS (SPFGMR, SPBCG, and SPTFQMR). For full details, including usage instructions, see the header files `sundials_spgmr.h` and `sundials_iterative.h`.

The files comprising the SPGMR generic linear solver, and their locations in the SUNDIALS *srcdir*, are as follows:

- header files (located in *srcdir/include/sundials*)  
`sundials_spgmr.h`, `sundials_iterative.h`, `sundials_nvector.h`,

`sundials_types.h`, `sundials_math.h`, `sundials_config.h`

- source files (located in `srcdir/src/sundials`)  
`sundials_spgmr.c`, `sundials_iterative.c`, `sundials_nvector.c`

Only two of the preprocessing directives in the header file `sundials_config.h` are required to use the SPGMR package by itself:

- (required) definition of the precision of the SUNDIALS type `realtype`. One of the following lines must be present:  

```
#define SUNDIALS_DOUBLE_PRECISION 1
#define SUNDIALS_SINGLE_PRECISION 1
#define SUNDIALS_EXTENDED_PRECISION 1
```
- (optional) use of generic math functions:  

```
#define SUNDIALS_USE_GENERIC_MATH 1
```

The `sundials_types.h` header file defines the SUNDIALS `realtype` and `booleantype` types and the macro `RCONST`, while the `sundials_math.h` header file is needed for the macros `SUNMIN`, `SUNMAX`, and `SUNSQR`, and the functions `SUNRabs` and `SUNRsqr`.

The generic `NVECTOR` files, `sundials_nvector.(h,c)` are needed for the definition of the generic `N_Vector` type and functions. The `NVECTOR` functions used by the SPGMR module are: `N_VDotProd`, `N_VLinearSum`, `N_VScale`, `N_VProd`, `N_VDiv`, `N_VConst`, `N_VClone`, `N_VCloneVectorArray`, `N_VDestroy`, and `N_VDestroyVectorArray`.

The nine files listed above can be extracted from the SUNDIALS `srcdir` and compiled by themselves into an SPGMR library or into a larger user code.

The following functions are available in the SPGMR package:

- `SpgmrMalloc`: allocation of memory for `SpgmrSolve`;
- `SpgmrSolve`: solution of  $Ax = b$  by the SPGMR method;
- `SpgmrFree`: free memory allocated by `SpgmrMalloc`.

The following functions are available in the support package `sundials_iterative.(h,c)`:

- `ModifiedGS`: performs modified Gram-Schmidt procedure;
- `ClassicalGS`: performs classical Gram-Schmidt procedure;
- `QRfact`: performs QR factorization of Hessenberg matrix;
- `QRsol`: solves a least squares problem with a Hessenberg matrix factored by `QRfact`.

### 8.3.2 The SPFGMR module

The SPFGMR package, in the files `sundials_spfgmr.h` and `sundials_spfgmr.c`, includes an implementation of the scaled preconditioned Flexible GMRES method. For full details, including usage instructions, see the file `sundials_spfgmr.h`.

The files needed to use the SPFGMR module by itself are the same as for the SPGMR module, but with `sundials_spfgmr.(h,c)` in place of `sundials_spgmr.(h,c)`.

The following functions are available in the SPFGMR package:

- `SpfgmrMalloc`: allocation of memory for `SpfgmrSolve`;
- `SpfgmrSolve`: solution of  $Ax = b$  by the SPFGMR method;
- `SpfgmrFree`: free memory allocated by `SpfgmrMalloc`.

### 8.3.3 The SPBCG module

The SPBCG package, in the files `sundials_spgmr.h` and `sundials_spgmr.c`, includes an implementation of the scaled preconditioned Bi-CGStab method. For full details, including usage instructions, see the file `sundials_spgmr.h`.

The files needed to use the SPBCG module by itself are the same as for the SPGMR module, but with `sundials_spgmr.h(c)` in place of `sundials_spgmr.h(c)`.

The following functions are available in the SPBCG package:

- `SpgmrMalloc`: allocation of memory for `SpgmrSolve`;
- `SpgmrSolve`: solution of  $Ax = b$  by the SPBCG method;
- `SpgmrFree`: free memory allocated by `SpgmrMalloc`.

### 8.3.4 The SPTFQMR module

The SPTFQMR package, in the files `sundials_sptfqr.h` and `sundials_sptfqr.c`, includes an implementation of the scaled preconditioned TFQMR method. For full details, including usage instructions, see the file `sundials_sptfqr.h`.

The files needed to use the SPTFQMR module by itself are the same as for the SPGMR module, but with `sundials_sptfqr.h(c)` in place of `sundials_spgmr.h(c)`.

The following functions are available in the SPTFQMR package:

- `SptfqrMalloc`: allocation of memory for `SptfqrSolve`;
- `SptfqrSolve`: solution of  $Ax = b$  by the SPTFQMR method;
- `SptfqrFree`: free memory allocated by `SptfqrMalloc`.

## 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 on 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 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.

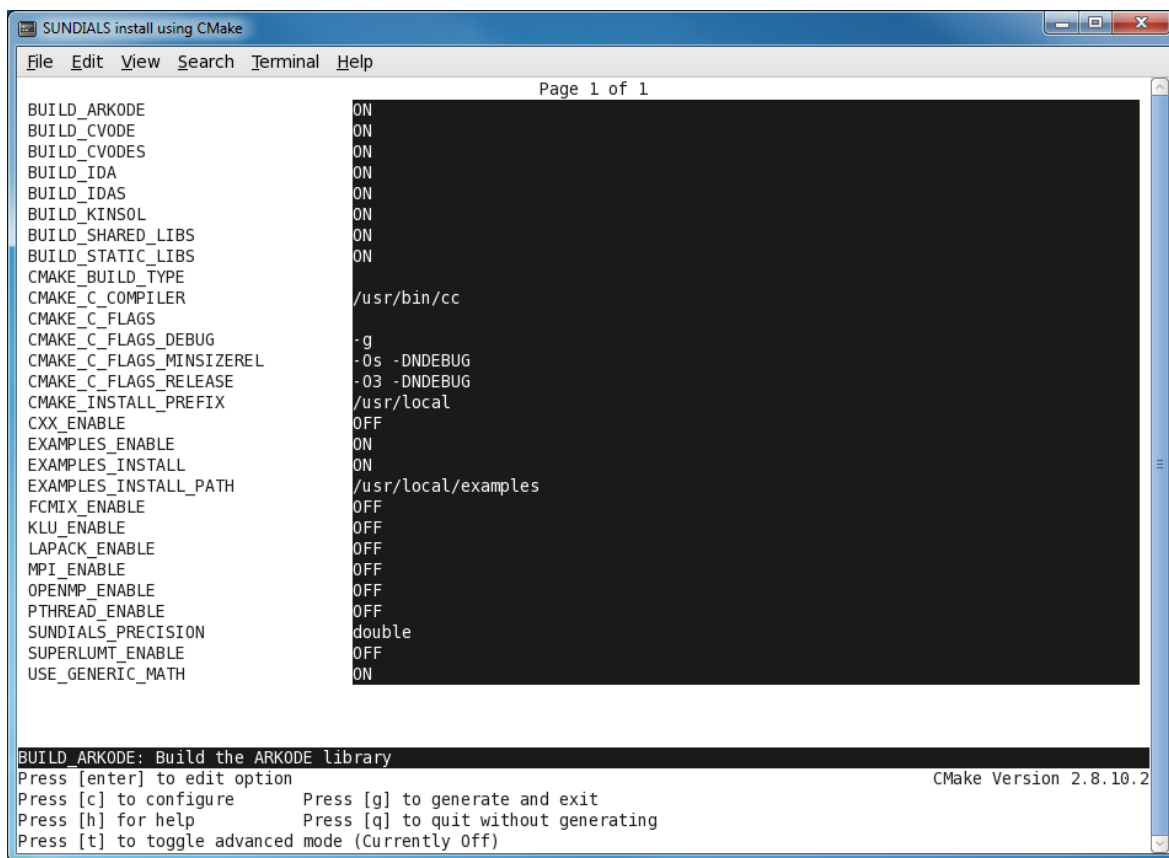


Figure A.1: Default configuration screen. Note: Initial screen is empty. To get this default configuration, press 'c' repeatedly (accepting default values denoted with asterisk) until the 'g' option is available.

The default *instldir* 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
```

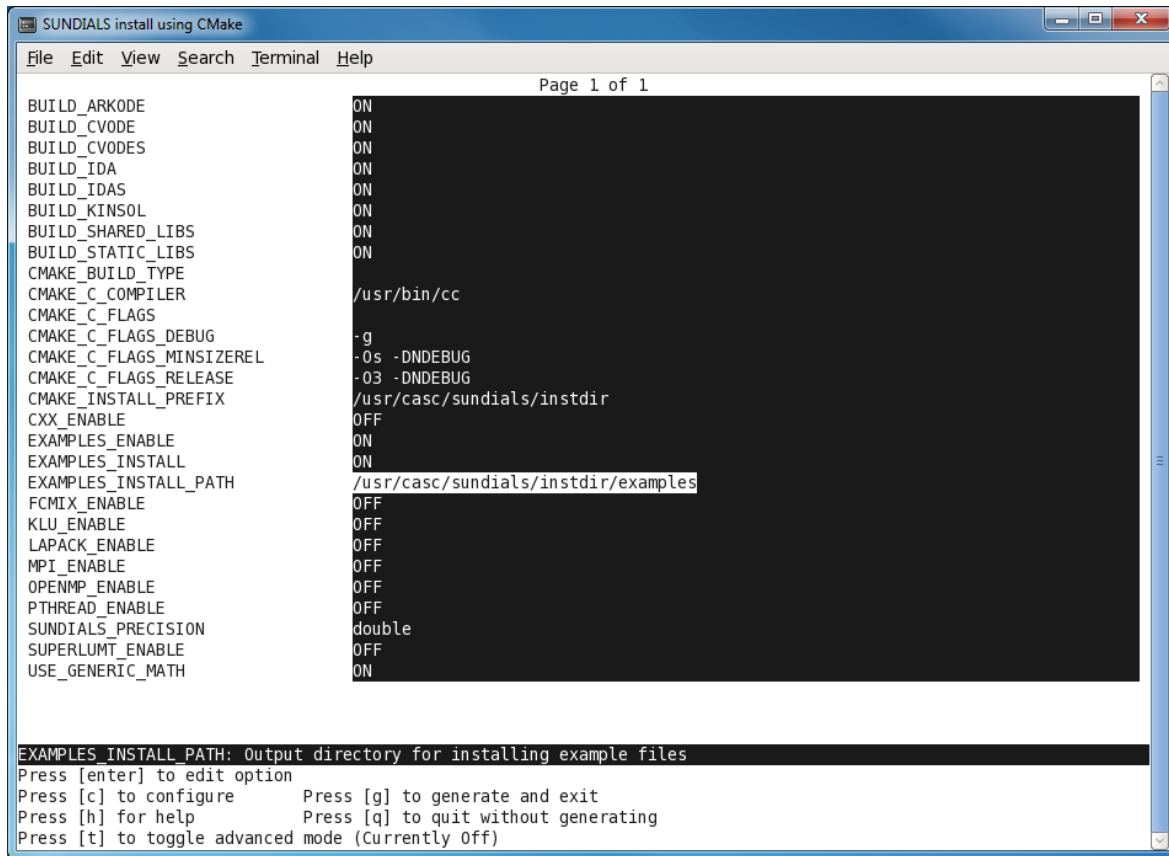


Figure A.2: Changing the *instdir* for SUNDIALS and corresponding examples

## 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.

**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: OFF
- 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 MinSizeRel  
Default:
- 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 compiler during debug builds  
Default: -g
- CMAKE\_C\_FLAGS\_MINSIZEREL** - Flags used by the compiler during release minsize builds  
Default: -Os -DNDEBUG
- CMAKE\_C\_FLAGS\_RELEASE** - Flags used by the 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 (LAPACK\_ENABLE is ON).
- CMAKE\_Fortran\_FLAGS** - Flags for Fortran compiler  
Default:
- CMAKE\_Fortran\_FLAGS\_DEBUG** - Flags used by the compiler during debug builds  
Default:
- CMAKE\_Fortran\_FLAGS\_MINSIZEREL** - Flags used by the compiler during release minsize builds  
Default:
- CMAKE\_Fortran\_FLAGS\_RELEASE** - Flags used by the compiler during release builds  
Default:
- 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.
- EXAMPLES\_ENABLE** - Build the SUNDIALS examples  
Default: ON

**EXAMPLES\_INSTALL** - Install example files

Default: ON

Note: This option is triggered only if building example programs is enabled (**EXAMPLES\_ENABLE** 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 have an **examples** subdirectory created under **CMAKE\_INSTALL\_PREFIX**.

**FCMIX\_ENABLE** - Enable Fortran-C support

Default: OFF

**HYPRE\_ENABLE** - Enable hypre support

Default: OFF

**HYPRE\_INCLUDE\_DIR** - Path to hypre header files

**HYPRE\_LIBRARY** - Path to hypre installed library

**KLU\_ENABLE** - Enable KLU support

Default: OFF

**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 the two additional options see below.

**LAPACK\_LIBRARIES** - Lapack (and Blas) libraries

Default: /usr/lib/liblapack.so;/usr/lib/libblas.so

Note: CMake will search for these libraries in your **LD\_LIBRARY\_PATH** prior to searching default system paths.

**MPI\_ENABLE** - Enable MPI support

Default: OFF

Note: Setting this option to ON will trigger several additional options related to MPI.

**MPI\_MPICC** - mpicc program

Default:

**MPI\_RUN\_COMMAND** - Specify run command for MPI

Default: mpirun

Note: This can either be set to **mpirun** for OpenMPI or **srun** if jobs are managed by **SLURM** - Simple Linux Utility for Resource Management as exists on LLNL's high performance computing clusters.

**MPI\_MPIF77** - mpif77 program

Default:

Note: This option is triggered only if using MPI compiler scripts (**MPI\_USE\_MPISCRIPTS** is ON) and Fortran-C support is enabled (**FCMIX\_ENABLE** is ON).

OPENMP\_ENABLE - Enable OpenMP support

Default: OFF

Turn on support for the OpenMP based nvector.

PETSC\_ENABLE - Enable PETSc support

Default: OFF

PETSC\_INCLUDE\_DIR - Path to PETSc header files

PETSC\_LIBRARY\_DIR - Path to PETSc installed library files

PTHREAD\_ENABLE - Enable Pthreads support

Default: OFF

Turn on support for the Pthreads based nvector.

SUNDIALS\_PRECISION - Precision used in SUNDIALS, options are: double, single or extended

Default: double

SUPERLUMT\_ENABLE - Enable SUPERLU\_MT support

Default: OFF

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

USE\_GENERIC\_MATH - Use generic (stdc) math libraries

Default: ON

### 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.

#### Building with LAPACK and BLAS

To enable LAPACK and BLAS libraries, set the `LAPACK_ENABLE` option to `ON`. If the directory containing the LAPACK and BLAS libraries is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `LAPACK_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the LAPACK and BLAS libraries in standard system locations. To explicitly tell CMake what libraries to use, the `LAPACK_LIBRARIES` variable can be set to the desired libraries. Example:

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DLAPACK_LIBRARIES=/mypath/lib/liblapack.so;/mypath/lib/libblas.so \
> /home/myname/sundials/srcdir
%
% make install
%
```

#### 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-scalable-linear-solvers-multigrid-methods>.

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.

## 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 both `EXAMPLES_ENABLE` and `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 Tables [A.1](#) and [A.2](#). 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_types.h
		sundials/sundials_math.h	
		sundials/sundials_nvector.h	sundials/sundials_fnvector.h
		sundials/sundials_direct.h	sundials/sundials_lapack.h
		sundials/sundials_dense.h	sundials/sundials_band.h
		sundials/sundials_sparse.h	
		sundials/sundials_iterative.h	sundials/sundials_spgmr.h
		sundials/sundials_spgbcs.h	sundials/sundials_sptfqmr.h
sundials/sundials_pcg.h	sundials/sundials_spgfmr.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	
CVMODE	Libraries	libsundials_cvmode. <i>lib</i>	libsundials_fcvmode.a
	Header files	cvmode/cvmode.h	cvmode/cvmode_impl.h
		cvmode/cvmode_direct.h	cvmode/cvmode_lapack.h
		cvmode/cvmode_dense.h	cvmode/cvmode_band.h
		cvmode/cvmode_diag.h	
		cvmode/cvmode_sparse.h	cvmode/cvmode_klu.h
		cvmode/cvmode_superlumt.h	
		cvmode/cvmode_spils.h	cvmode/cvmode_spgmr.h
		cvmode/cvmode_sptfqmr.h	cvmode/cvmode_spgbcs.h
cvmode/cvmode_bandpre.h	cvmode/cvmode_bbdpre.h		
CVMODES	Libraries	libsundials_cvmodes. <i>lib</i>	
	Header files	cvmodes/cvmodes.h	cvmodes/cvmodes_impl.h
		cvmodes/cvmodes_direct.h	cvmodes/cvmodes_lapack.h
		cvmodes/cvmodes_dense.h	cvmodes/cvmodes_band.h
		cvmodes/cvmodes_diag.h	
		cvmodes/cvmodes_sparse.h	cvmodes/cvmodes_klu.h
		cvmodes/cvmodes_superlumt.h	
		cvmodes/cvmodes_spils.h	cvmodes/cvmodes_spgmr.h
		cvmodes/cvmodes_sptfqmr.h	cvmodes/cvmodes_spgbcs.h
cvmodes/cvmodes_bandpre.h	cvmodes/cvmodes_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_lapack.h
		arkode/arkode_dense.h	arkode/arkode_band.h
		arkode/arkode_sparse.h	arkode/arkode_klu.h
		arkode/arkode_superlumt.h	
		arkode/arkode_spils.h	arkode/arkode_spgmr.h
		arkode/arkode_sptfqmr.h	arkode/arkode_spgbcs.h
		arkode/arkode_pcg.h	arkode/arkode_spgfmr.h
arkode/arkode_bandpre.h	arkode/arkode_bbdpre.h		

Table A.2: SUNDIALS libraries and header files (cont.)

IDA	Libraries	libsundials_ida. <i>lib</i>	libsundials_fida.a
	Header files	ida/ida.h ida/ida_direct.h ida/ida_dense.h ida/ida_sparse.h ida/ida_superlunt.h ida/ida_spils.h ida/ida_spgmr.h ida/ida_sptfqmr.h	ida/ida_impl.h ida/ida_lapack.h ida/ida_band.h ida/ida_klu.h ida/ida_spgmr.h ida/ida_sptfqmr.h
IDAS	Libraries	libsundials_idas. <i>lib</i>	
	Header files	idas/idas.h idas/idas_direct.h idas/idas_dense.h idas/idas_sparse.h idas/idas_superlunt.h idas/idas_spils.h idas/idas_spgmr.h idas/idas_sptfqmr.h	idas/idas_impl.h idas/idas_lapack.h idas/idas_band.h idas/idas_klu.h idas/idas_spgmr.h idas/idas_sptfqmr.h
KINSOL	Libraries	libsundials_kinsol. <i>lib</i>	libsundials_fkinsol.a
	Header files	kinsol/kinsol.h kinsol/kinsol_direct.h kinsol/kinsol_dense.h kinsol/kinsol_sparse.h kinsol/kinsol_superlunt.h kinsol/kinsol_spils.h kinsol/kinsol_spgmr.h kinsol/kinsol_sptfqmr.h	kinsol/kinsol_impl.h kinsol/kinsol_lapack.h kinsol/kinsol_band.h kinsol/kinsol_klu.h kinsol/kinsol_spgmr.h kinsol/kinsol_sptfqmr.h kinsol/kinsol_sptfqmr.h

# Appendix B

## CVODE Constants

Below we list all input and output constants used by the main solver and linear solver modules, together with their numerical values and a short description of their meaning.

### B.1 CVODE input constants

CVODE main solver module		
CV_ADAMS	1	Adams-Moulton linear multistep method.
CV_BDF	2	BDF linear multistep method.
CV_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.
Iterative linear solver module		
PREC_NONE	0	No preconditioning
PREC_LEFT	1	Preconditioning on the left only.
PREC_RIGHT	2	Preconditioning on the right only.
PREC_BOTH	3	Preconditioning on both the left and the right.
MODIFIED_GS	1	Use modified Gram-Schmidt procedure.
CLASSICAL_GS	2	Use classical Gram-Schmidt procedure.

### B.2 CVODE output constants

CVODE main solver module		
CV_SUCCESS	0	Successful function return.
CV_TSTOP_RETURN	1	CVode succeeded by reaching the specified stopping point.
CV_ROOT_RETURN	2	CVode succeeded and found one or more roots.
CV_WARNING	99	CVode succeeded but an unusual situation occurred.
CV_TOO_MUCH_WORK	-1	The solver took <code>mxstep</code> internal steps but could not reach tout.

CV_TOO_MUCH_ACC	-2	The solver could not satisfy the accuracy demanded by the user for some internal step.
CV_ERR_FAILURE	-3	Error test failures occurred too many times during one internal time step or minimum step size was reached.
CV_CONV_FAILURE	-4	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
CV_LINIT_FAIL	-5	The linear solver's initialization function failed.
CV_LSETUP_FAIL	-6	The linear solver's setup function failed in an unrecoverable manner.
CV_LSOLVE_FAIL	-7	The linear solver's solve function failed in an unrecoverable manner.
CV_RHSFUNC_FAIL	-8	The right-hand side function failed in an unrecoverable manner.
CV_FIRST_RHSFUNC_ERR	-9	The right-hand side function failed at the first call.
CV_REPTD_RHSFUNC_ERR	-10	The right-hand side function had repeated recoverable errors.
CV_UNREC_RHSFUNC_ERR	-11	The right-hand side function had a recoverable error, but no recovery is possible.
CV_RTFUNC_FAIL	-12	The rootfinding function failed in an unrecoverable manner.
CV_MEM_FAIL	-20	A memory allocation failed.
CV_MEM_NULL	-21	The <code>cvode_mem</code> argument was NULL.
CV_ILL_INPUT	-22	One of the function inputs is illegal.
CV_NO_MALLOC	-23	The CVODE memory block was not allocated by a call to <code>CVodeMalloc</code> .
CV_BAD_K	-24	The derivative order $k$ is larger than the order used.
CV_BAD_T	-25	The time $t$ is outside the last step taken.
CV_BAD_DKY	-26	The output derivative vector is NULL.
CV_TOO_CLOSE	-27	The output and initial times are too close to each other.

---

**CVDSL linear solver modules**


---

CVDSL_SUCCESS	0	Successful function return.
CVDSL_MEM_NULL	-1	The <code>cvode_mem</code> argument was NULL.
CVDSL_LMEM_NULL	-2	The CVDSL linear solver has not been initialized.
CVDSL_ILL_INPUT	-3	The CVDSL solver is not compatible with the current NVECTOR module.
CVDSL_MEM_FAIL	-4	A memory allocation request failed.
CVDSL_JACFUNC_UNRECVR	-5	The Jacobian function failed in an unrecoverable manner.
CVDSL_JACFUNC_RECVR	-6	The Jacobian function had a recoverable error.

---

**CVDIAG linear solver module**


---

CVDIAG_SUCCESS	0	Successful function return.
CVDIAG_MEM_NULL	-1	The <code>cvode_mem</code> argument was NULL.
CVDIAG_LMEM_NULL	-2	The CVDIAG linear solver has not been initialized.

CVDIAG_ILL_INPUT	-3	The CVDIAG solver is not compatible with the current NVECTOR module.
CVDIAG_MEM_FAIL	-4	A memory allocation request failed.
CVDIAG_INV_FAIL	-5	A diagonal element of the Jacobian was 0.
CVDIAG_RHSFUNC_UNRECV	-6	The right-hand side function failed in an unrecoverable manner.
CVDIAG_RHSFUNC_RECV	-7	The right-hand side function had a recoverable error.
<hr/> <b>CVSLS linear solver module</b> <hr/>		
CVSLS_SUCCESS	0	Successful function return.
CVSLS_MEM_NULL	-1	The <code>cv_mem</code> argument was NULL.
CVSLS_LMEM_NULL	-2	The CVSLS linear solver has not been initialized.
CVSLS_ILL_INPUT	-3	The CVSLS solver is not compatible with the current NVECTOR module or other input is invalid.
CVSLS_MEM_FAIL	-4	A memory allocation request failed.
CVSLS_JAC_NOSET	-5	The Jacobian evaluation routine was not been set before the linear solver setup routine was called.
CVSLS_PACKAGE_FAIL	-6	An external package call return a failure error code.
CVSLS_JACFUNC_UNRECV	-7	The Jacobian function failed in an unrecoverable manner.
CVSLS_JACFUNC_RECV	-8	The Jacobian function had a recoverable error.
<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.
<hr/> <b>SPGMR generic linear solver module</b> <hr/>		
SPGMR_SUCCESS	0	Converged.
SPGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPGMR_CONV_FAIL	2	Failure to converge.
SPGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPGMR_ATIMES_FAIL_REC	5	The Jacobian-times-vector function failed recoverably.
SPGMR_PSET_FAIL_REC	6	The preconditioner setup routine failed recoverably.
SPGMR_MEM_NULL	-1	The SPGMR memory is NULL
SPGMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.

SPGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPGMR_QRSOL_FAIL	-5	The matrix $R$ was found to be singular during the QR solve phase.
SPGMR_PSET_FAIL_UNREC	-6	The preconditioner setup routine failed unrecoverably.

---

**SPFGMR generic linear solver module (only available in KINSOL and ARKODE)**

---

SPFGMR_SUCCESS	0	Converged.
SPFGMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPFGMR_CONV_FAIL	2	Failure to converge.
SPFGMR_QRFACT_FAIL	3	A singular matrix was found during the QR factorization.
SPFGMR_PSOLVE_FAIL_REC	4	The preconditioner solve function failed recoverably.
SPFGMR_ATIMES_FAIL_REC	5	The Jacobian-times-vector function failed recoverably.
SPFGMR_PSET_FAIL_REC	6	The preconditioner setup routine failed recoverably.
SPFGMR_MEM_NULL	-1	The SPFGMR memory is NULL
SPFGMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPFGMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPFGMR_GS_FAIL	-4	Failure in the Gram-Schmidt procedure.
SPFGMR_QRSOL_FAIL	-5	The matrix $R$ was found to be singular during the QR solve phase.
SPFGMR_PSET_FAIL_UNREC	-6	The preconditioner setup routine failed unrecoverably.

---

**SPBCG generic linear solver module**

---

SPBCG_SUCCESS	0	Converged.
SPBCG_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPBCG_CONV_FAIL	2	Failure to converge.
SPBCG_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPBCG_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPBCG_PSET_FAIL_REC	5	The preconditioner setup routine failed recoverably.
SPBCG_MEM_NULL	-1	The SPBCG memory is NULL
SPBCG_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed unrecoverably.
SPBCG_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPBCG_PSET_FAIL_UNREC	-4	The preconditioner setup routine failed unrecoverably.

---

**SPTFQMR generic linear solver module**

---

SPTFQMR_SUCCESS	0	Converged.
SPTFQMR_RES_REDUCED	1	No convergence, but the residual norm was reduced.
SPTFQMR_CONV_FAIL	2	Failure to converge.
SPTFQMR_PSOLVE_FAIL_REC	3	The preconditioner solve function failed recoverably.
SPTFQMR_ATIMES_FAIL_REC	4	The Jacobian-times-vector function failed recoverably.
SPTFQMR_PSET_FAIL_REC	5	The preconditioner setup routine failed recoverably.
SPTFQMR_MEM_NULL	-1	The SPTFQMR memory is NULL

---

SPTFQMR_ATIMES_FAIL_UNREC	-2	The Jacobian-times-vector function failed.
SPTFQMR_PSOLVE_FAIL_UNREC	-3	The preconditioner solve function failed unrecoverably.
SPTFQMR_PSET_FAIL_UNREC	-4	The preconditioner setup routine failed unrecoverably.



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