User Documentation for CVODE v6.7.0

SUNDIALS v6.7.0

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The SUNDIALS library has been developed over many years by a number of contributors. The current SUNDIALS team consists of Cody J. Balos, David J. Gardner, Alan C. Hindmarsh, Daniel R. Reynolds, and Carol S. Woodward. We thank Radu Serban for significant and critical past contributions.

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Chapter 1

Introduction

CVODE is part of a software family called SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic equation Solvers [38]. 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 [14] and VODPK [17]. VODE is a general purpose solver that includes methods for both stiff and nonstiff systems, and in the stiff case uses direct methods (full or banded) for the solution of the linear systems that arise at each implicit step. Externally, VODE is very similar to the well known solver LSODE [48]. 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 [15]. The capabilities of both VODE and VODPK have been combined in the C-language package CVODE [22].

At present, CVODE may utilize a variety of Krylov methods provided in SUNDIALS that can be used in conjuction with Newton iteration: these include the GMRES (Generalized Minimal RESidual) [50], FGMRES (Flexible Generalized Minimum RESidual) [49], Bi-CGStab (Bi-Conjugate Gradient Stabilized) [56], TFQMR (Transpose-Free Quasi-Minimal Residual) [31], and PCG (Preconditioned Conjugate Gradient) [33] linear iterative methods. As Krylov methods, these require almost no matrix storage for solving the Newton equations as compared to direct methods. However, the algorithms allow for a user-supplied preconditioner matrix, and for most problems preconditioning is essential for an efficient solution. For very large stiff ODE systems, the Krylov methods are preferable over direct linear solver methods, and are often the only feasible choice. Among the Krylov methods in SUNDIALS, we recommend GMRES as the best overall choice. However, users are encouraged to compare all options, especially if encountering convergence failures with GMRES. Bi-CGStab and TFQMR have an advantage in storage requirements, in that the number of workspace vectors they require is fixed, while that number for GMRES depends on the desired Krylov subspace size. FGMRES has an advantage in that it is designed to support preconditioners that vary between iterations (e.g. iterative methods). PCG exhibits rapid convergence and minimal workspace vectors, but only works for symmetric linear systems.

In the process of translating the VODE and VODPK algorithms into C, the overall CVODE organization has been changed considerably. One key feature of the CVODE organization is that the linear system solvers comprise a layer of code modules that is separated from the integration algorithm, allowing for easy modification and expansion of the linear solver array. A second key feature is a separate module devoted to vector operations; this facilitated the extension to multiprosessor environments with minimal impacts on the rest of the solver, resulting in PVODE [20], the parallel variant of CVODE.

Around 2002, the functionality of CVODE and PVODE were combined into one single code, simply called CVODE. Development of this version of CVODE was concurrent with a redesign of the vector operations module across the SUNDIALS suite. The key feature of the `N_Vector` 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 `N_Vector`. This allows writing the SUNDIALS solvers in a manner independent of the actual `N_Vector` implementation (which can be user-supplied), as well as allowing more than one `N_Vector` module linked into an executable file. SUNDIALS (and thus CVODE) is supplied with a wide range of different `N_Vector` implementations, including: serial, MPI-parallel, both OpenMP and Pthreads thread-parallel `N_Vector` implementations, a Hypre parallel implementation, a PETSc implementation, and various GPU-enabled implementations.

1.2 Changes from previous versions

1.2.1 Changes in v6.7.0

Improved computational complexity of `SUNMatScaleAddI_Sparse` from `O(M*N)` to `O(NNZ)`.

Added Fortran support for the LAPACK dense `SUNLinearSolver` implementation.

Fixed a regression introduced by the stop time bug fix in v6.6.1 where CVODE would return at the stop time rather than the requested output time if the stop time was reached in the same step in which the output time was passed.

Fixed scaling bug in `SUNMatScaleAddI_Sparse` for non-square matrices.

Changed the `SUNProfiler` so that it does not rely on `MPI_WTime` in any case. This fixes GitHub Issue #312.

Fixed missing soversions in some `SUNLinearSolver` and `SUNNonlinearSolver` CMake targets.

1.2.2 Changes in v6.6.2

Fixed the build system support for MAGMA when using a NVIDIA HPC SDK installation of CUDA and fixed the targets used for rocBLAS and rocSPARSE.

1.2.3 Changes in v6.6.1

Updated the Tpetra NVector interface to support Trilinos 14.

Fixed a memory leak when destroying a CUDA, HIP, SYCL, or system SUNMemoryHelper object.

Fixed a bug where the stop time may not be cleared when using normal mode if the requested output time is the same as the stop time. Additionally, this fix removes an unnecessary interpolation of the solution at the stop time that could occur in this case.

1.2.4 Changes in v6.6.0

Updated the default CVODE behavior when returning the solution when the internal time has reached a user-specified stop time. Previously, the output solution was interpolated to the value of `tstop`; the default is now to copy the internal solution vector. Users who wish to revert to interpolation may call the routine *CVodeSetInterpolateStopTime()*.

Updated the F2003 utility routines *SUNDIALSFileOpen()* and *SUNDIALSFileClose()* to support user specification of `stdout` and `stderr` strings for the output file names.

1.2.5 Changes in v6.5.1

Added the function *CVodeClearStopTime()* to disable a previously set stop time.

Fixed build errors when using SuperLU_DIST with ROCM enabled to target AMD GPUs.

Fixed compilation errors in some SYCL examples when using the `icx` compiler.

1.2.6 Changes in v6.5.0

Added the functions *CVodeGetJac()*, *CVodeGetJacTime()*, *CVodeGetJacNumSteps()* to assist in debugging simulations utilizing a matrix-based linear solver.

Added support for the SYCL backend with RAJA 2022.x.y.

Fixed an underflow bug during root finding.

A new capability to keep track of memory allocations made through the `SUNMemoryHelper` classes has been added. Memory allocation stats can be accessed through the *SUNMemoryHelper_GetAllocStats()* function. See the documentation for the `SUNMemoryHelper` classes for more details.

Added support for CUDA v12. Fixed an issue with finding oneMKL when using the `icpx` compiler with the `-fsycl` flag as the C++ compiler instead of `dpcpp`.

Fixed the shape of the arrays returned by `FN_VGetArrayPointer` functions as well as the `FSUNDenseMatrix_-Data`, `FSUNBandMatrix_Data`, `FSUNSparseMatrix_Data`, `FSUNSparseMatrix_IndexValues`, and `FSUNSparse-Matrix_IndexPointers` functions. Compiling and running code that uses the SUNDIALS Fortran interfaces with bounds checking will now work.

1.2.7 Changes in v6.4.1

Fixed a bug with the Kokkos interfaces that would arise when using clang.

Fixed a compilation error with the Intel oneAPI 2022.2 Fortran compiler in the Fortran 2003 interface test for the serial `N_Vector`.

Fixed a bug in the SUNLINSOL_LAPACKBAND and SUNLINSOL_LAPACKDENSE modules which would cause the tests to fail on some platforms.

1.2.8 Changes in v6.4.0

CMake 3.18.0 or newer is now required for CUDA support.

A C++14 compliant compiler is now required for C++ based features and examples e.g., CUDA, HIP, RAJA, Trilinos, SuperLU_DIST, MAGMA, GINKGO, and KOKKOS.

Added support for GPU enabled SuperLU_DIST and SuperLU_DIST v8.x.x. Removed support for SuperLU_DIST v6.x.x or older. Fix mismatched definition and declaration bug in SuperLU_DIST matrix constructor.

Added support for the Ginkgo linear algebra library. This support includes new `SUNMatrix` and `SUNLinearSolver` implementations, see the sections §7.10 and §8.18.

Added new `NVector`, dense `SUNMatrix`, and dense `SUNLinearSolver` implementations utilizing the Kokkos Ecosystem for performance portability, see sections §6.14, §7.11, and §8.19 for more information.

Fixed a bug in the CUDA and HIP vectors where *N_VMaxNorm()* would return the minimum positive floating-point value for the zero vector.

Fixed a memory leak where the projection memory would not be deallocated when calling *CVodeFree()*.

1.2.9 Changes in v6.3.0

Added the function *CVodeGetUserData()* to retrieve the user data pointer provided to *CVodeSetUserData()*.

Added a new example, `examples/cvode/serial/cvRocket_dns.c`, which demonstrates using CVODE with a discontinuous right-hand-side function and rootfinding.

Fixed the unitutive behavior of the *USE_GENERIC_MATH* CMake option which caused the double precision math functions to be used regardless of the value of *SUNDIALS_PRECISION*. Now, SUNDIALS will use precision appropriate math functions when they are available and the user may provide the math library to link to via the advanced CMake option *SUNDIALS_MATH_LIBRARY*.

Changed *SUNDIALS_LOGGING_ENABLE_MPI* CMake option default to be 'OFF'.

1.2.10 Changes in v6.2.0

Added the *SUNLogger* API which provides a SUNDIALS-wide mechanism for logging of errors, warnings, informational output, and debugging output.

Deprecated *SUNNonlinSolSetPrintLevel_Newton()*, *SUNNonlinSolSetInfoFile_Newton()*, *SUNNonlinSolSetPrintLevel_FixedPoint()*, *SUNNonlinSolSetInfoFile_FixedPoint()*, *SUNLinSolSetInfoFile_PCG()*, *SUNLinSolSetPrintLevel_PCG()*, *SUNLinSolSetInfoFile_SPGMR()*, *SUNLinSolSetPrintLevel_SPGMR()*, *SUNLinSolSetInfoFile_SPFGMR()*, *SUNLinSolSetPrintLevel_SPFGMR()*, SUNLinSolSetInfoFile_SPTFQM(), *SUNLinSolSetPrintLevel_SPTFQMR()*, *SUNLinSolSetInfoFile_SPBCGS()*, *SUNLinSolSetPrintLevel_SPBCGS()* it is recommended to use the *SUNLogger* API instead. The SUNLinSolSetInfoFile_** and SUNNonlinSolSetInfoFile_* family of functions are now enabled by setting the CMake option *SUNDIALS_LOGGING_LEVEL* to a value >= 3.

Added the function *SUNProfiler_Reset()* to reset the region timings and counters to zero.

Added the function *CVodePrintAllStats()* to output all of the integrator, nonlinear solver, linear solver, and other statistics in one call. The file `scripts/sundials_csv.py` contains functions for parsing the comma-separated value output files.

Added the functions *CVodeSetEtaFixedStepBounds()*, *CVodeSetEtaMaxFirstStep()*, *CVodeSetEtaMaxEarlyStep()*, *CVodeSetNumStepsEtaMaxEarlyStep()*, *CVodeSetEtaMax()*, *CVodeSetEtaMin()*, *CVodeSetEtaMinErrFail()*, *CVodeSetEtaMaxErrFail()*, *CVodeSetNumFailsEtaMaxErrFail()*, and *CVodeSetEtaConvFail()* to adjust various parameters controlling changes in step size.

Added the functions *CVodeSetDeltaGammaMaxLSetup()* and *CVodeSetDeltaGammaMaxBadJac()* to adjust the γ change thresholds to require a linear solver setup or Jacobian/precondition update, respectively.

The behavior of N_VSetKernelExecPolicy_Sycl() has been updated to be consistent with the CUDA and HIP vectors. The input execution policies are now cloned and may be freed after calling N_VSetKernelExecPolicy_Sycl(). Additionally, NULL inputs are now allowed and, if provided, will reset the vector execution policies to the defaults.

Fixed the *SUNContext* convenience class for C++ users to disallow copy construction and allow move construction.

A memory leak in the SYCL vector was fixed where the execution policies were not freed when the vector was destroyed.

The include guard in nvector_mpimanyvector.h has been corrected to enable using both the ManyVector and MPI-ManyVector NVector implementations in the same simulation.

Changed exported SUNDIALS PETSc CMake targets to be INTERFACE IMPORTED instead of UNKNOWN IMPORTED.

A bug was fixed in the functions *CVodeGetNumNonlinSolvConvFails()* and *CVodeGetNonlinSolvStats()* where the number of nonlinear solver failures returned was the number of failed *steps* due to a nonlinear solver failure i.e., if

a nonlinear solve failed with a stale Jacobian or preconditioner but succeeded after updating the Jacobian or precon-
ditioner, the initial failure was not included in the nonlinear solver failure count. These functions have been updated
to return the total number of nonlinear solver failures. As such users may see an increase in the number of failures
reported.

The function `CVodeGetNumStepSolveFails()` has been added to retrieve the number of failed steps due to a nonlinear
solver failure. The count returned by this function will match those previously returned by `CVodeGetNumNonlinSolv-`
`ConvFails()` and `CVodeGetNonlinSolvStats()`.

1.2.11 Changes in v6.1.1

Fixed exported `SUNDIALSConfig.cmake`.

1.2.12 Changes in v6.1.0

Added new reduction implementations for the CUDA and HIP NVECTORs that use shared memory (local data storage)
instead of atomics. These new implementations are recommended when the target hardware does not provide atomic
support for the floating point precision that SUNDIALS is being built with. The HIP vector uses these by default, but
the `N_VSetKernelExecPolicy_Cuda()` and `N_VSetKernelExecPolicy_Hip()` functions can be used to choose
between different reduction implementations.

`SUNDIALS::<lib>` targets with no static/shared suffix have been added for use within the build directory (this mirrors
the targets exported on installation).

`CMAKE_C_STANDARD` is now set to 99 by default.

Fixed exported `SUNDIALSConfig.cmake` when profiling is enabled without Caliper.

Fixed `sundials_export.h` include in `sundials_config.h`.

Fixed memory leaks in the SUNLINSOL_SUPERLUMT linear solver.

1.2.13 Changes in v6.0.0

SUNContext

SUNDIALS v6.0.0 introduces a new `SUNContext` object on which all other SUNDIALS objects depend. As such, the
constructors for all SUNDIALS packages, vectors, matrices, linear solvers, nonlinear solvers, and memory helpers
have been updated to accept a context as the last input. Users upgrading to SUNDIALS v6.0.0 will need to call
`SUNContext_Create()` to create a context object with before calling any other SUNDIALS library function, and then
provide this object to other SUNDIALS constructors. The context object has been introduced to allow SUNDIALS to
provide new features, such as the profiling/instrumentation also introduced in this release, while maintaining thread-
safety. See the documentation section on the `SUNContext` for more details.

A script `upgrade-to-sundials-6-from-5.sh` has been provided with the release (obtainable from the GitHub re-
lease page) to help ease the transition to SUNDIALS v6.0.0. The script will add a `SUNCTX_PLACEHOLDER` argument
to all of the calls to SUNDIALS constructors that now require a `SUNContext` object. It can also update deprecated
SUNDIALS constants/types to the new names. It can be run like this:

```
> ./upgrade-to-sundials-6-from-5.sh <files to update>
```

SUNProfiler

A capability to profile/instrument SUNDIALS library code has been added. This can be enabled with the CMake option
`SUNDIALS_BUILD_WITH_PROFILING`. A built-in profiler will be used by default, but the Caliper library can also be

used instead with the CMake option *ENABLE_CALIPER*. See the documentation section on profiling for more details. **WARNING**: Profiling will impact performance, and should be enabled judiciously.

SUNMemoryHelper

The *SUNMemoryHelper* functions *SUNMemoryHelper_Alloc()*, *SUNMemoryHelper_Dealloc()*, and *SUNMemory-Helper_Copy()* have been updated to accept an opaque handle as the last input. At a minimum, user-defined *SUN-MemoryHelper* implementations will need to update these functions to accept the additional argument. Typically, this handle is the execution stream (e.g., a CUDA/HIP stream or SYCL queue) for the operation. The *CUDA*, *HIP*, and *SYCL* implementations have been updated accordingly. Additionally, the constructor *SUNMemoryHelper_Sycl()* has been updated to remove the SYCL queue as an input.

NVector

Two new optional vector operations, *N_VDotProdMultiLocal()* and *N_VDotProdMultiAllReduce()*, have been added to support low-synchronization methods for Anderson acceleration.

The CUDA, HIP, and SYCL execution policies have been moved from the `sundials` namespace to the `sundials::cuda`, `sundials::hip`, and `sundials::sycl` namespaces respectively. Accordingly, the prefixes "Cuda", "Hip", and "Sycl" have been removed from the execution policy classes and methods.

The `Sundials` namespace used by the Trilinos Tpetra NVector has been replaced with the `sundials::trilinos::nvector_tpetra` namespace.

The serial, PThreads, PETSc, *hypre*, Parallel, OpenMP_DEV, and OpenMP vector functions `N_VCloneVectorArray_*` and `N_VDestroyVectorArray_*` have been deprecated. The generic *N_VCloneVectorArray()* and *N_VDestroyVectorArray()* functions should be used instead.

The previously deprecated constructor `N_VMakeWithManagedAllocator_Cuda` and the function `N_VSetCudaStream_Cuda` have been removed and replaced with *N_VNewWithMemHelp_Cuda()* and `N_VSetKerrnelExecPolicy_Cuda()` respectively.

The previously deprecated macros `PVEC_REAL_MPI_TYPE` and `PVEC_INTEGER_MPI_TYPE` have been removed and replaced with `MPI_SUNREALTYPE` and `MPI_SUNINDEXTYPE` respectively.

SUNLinearSolver

The following previously deprecated functions have been removed:

Removed	Replacement
SUNBandLinearSolver	*SUNLinSol_Band()*
SUNDenseLinearSolver	*SUNLinSol_Dense()*
SUNKLU	*SUNLinSol_KLU()*
SUNKLUReInit	*SUNLinSol_KLUReInit()*
SUNKLUSetOrdering	*SUNLinSol_KLUSetOrdering()*
SUNLapackBand	*SUNLinSol_LapackBand()*
SUNLapackDense	*SUNLinSol_LapackDense()*
SUNPCG	*SUNLinSol_PCG()*
SUNPCGSetPrecType	*SUNLinSol_PCGSetPrecType()*
SUNPCGSetMaxl	*SUNLinSol_PCGSetMaxl()*
SUNSPBCGS	*SUNLinSol_SPBCGS()*
SUNSPBCGSSetPrecType	*SUNLinSol_SPBCGSSetPrecType()*
SUNSPBCGSSetMaxl	*SUNLinSol_SPBCGSSetMaxl()*
SUNSPFGMR	*SUNLinSol_SPFGMR()*
SUNSPFGMRSetPrecType	*SUNLinSol_SPFGMRSetPrecType()*
SUNSPFGMRSetGSType	*SUNLinSol_SPFGMRSetGSType()*
SUNSPFGMRSetMaxRestarts	*SUNLinSol_SPFGMRSetMaxRestarts()*
SUNSPGMR	*SUNLinSol_SPGMR()*
SUNSPGMRSetPrecType	*SUNLinSol_SPGMRSetPrecType()*
SUNSPGMRSetGSType	*SUNLinSol_SPGMRSetGSType()*
SUNSPGMRSetMaxRestarts	*SUNLinSol_SPGMRSetMaxRestarts()*
SUNSPTFQMR	*SUNLinSol_SPTFQMR()*
SUNSPTFQMRSetPrecType	*SUNLinSol_SPTFQMRSetPrecType()*
SUNSPTFQMRSetMaxl	*SUNLinSol_SPTFQMRSetMaxl()*
SUNSuperLUMT	*SUNLinSol_SuperLUMT()*
SUNSuperLUMTSetOrdering	*SUNLinSol_SuperLUMTSetOrdering()*

CVODE

The previously deprecated function CVodeSetMaxStepsBetweenJac has been removed and replaced with *CVode-SetJacEvalFrequency()*.

The CVODE Fortran 77 interface has been removed. See §4.5 and the F2003 example programs for more details using the SUNDIALS Fortran 2003 module interfaces.

Deprecations

In addition to the deprecations noted elsewhere, many constants, types, and functions have been renamed so that they are properly namespaced. The old names have been deprecated and will be removed in SUNDIALS v7.0.0.

The following constants, macros, and typedefs are now deprecated:

Deprecated Name	New Name
realtype	sunrealtype
booleantype	sunbooleantype
RCONST	SUN_RCONST
BIG_REAL	SUN_BIG_REAL
SMALL_REAL	SUN_SMALL_REAL
UNIT_ROUNDOFF	SUN_UNIT_ROUNDOFF
PREC_NONE	SUN_PREC_NONE
PREC_LEFT	SUN_PREC_LEFT
PREC_RIGHT	SUN_PREC_RIGHT
PREC_BOTH	SUN_PREC_BOTH
MODIFIED_GS	SUN_MODIFIED_GS
CLASSICAL_GS	SUN_CLASSICAL_GS
ATimesFn	SUNATimesFn
PSetupFn	SUNPSetupFn
PSolveFn	SUNPSolveFn
DlsMat	SUNDlsMat
DENSE_COL	SUNDLS_DENSE_COL
DENSE_ELEM	SUNDLS_DENSE_ELEM
BAND_COL	SUNDLS_BAND_COL
BAND_COL_ELEM	SUNDLS_BAND_COL_ELEM
BAND_ELEM	SUNDLS_BAND_ELEM

In addition, the following functions are now deprecated (compile-time warnings will be thrown if supported by the compiler):

Deprecated Name	New Name
CVSpilsSetLinearSolver	CVodeSetLinearSolver
CVSpilsSetEpsLin	CVodeSetEpsLin
CVSpilsSetPreconditioner	CVodeSetPreconditioner
CVSpilsSetJacTimes	CVodeSetJacTimes
CVSpilsGetWorkSpace	CVodeGetLinWorkSpace
CVSpilsGetNumPrecEvals	CVodeGetNumPrecEvals
CVSpilsGetNumPrecSolves	CVodeGetNumPrecSolves
CVSpilsGetNumLinIters	CVodeGetNumLinIters
CVSpilsGetNumConvFails	CVodeGetNumConvFails
CVSpilsGetNumJTSetupEvals	CVodeGetNumJTSetupEvals
CVSpilsGetNumJtimesEvals	CVodeGetNumJtimesEvals
CVSpilsGetNumRhsEvals	CVodeGetNumLinRhsEvals
CVSpilsGetLastFlag	CVodeGetLastLinFlag
CVSpilsGetReturnFlagName	CVodeGetLinReturnFlagName
CVDlsSetLinearSolver	CVodeSetLinearSolver
CVDlsSetJacFn	CVodeSetJacFn
CVDlsGetWorkSpace	CVodeGetLinWorkSpace
CVDlsGetNumJacEvals	CVodeGetNumJacEvals
CVDlsGetNumRhsEvals	CVodeGetNumLinRhsEvals
CVDlsGetLastFlag	CVodeGetLastLinFlag
CVDlsGetReturnFlagName	CVodeGetLinReturnFlagName
DenseGETRF	SUNDlsMat_DenseGETRF
DenseGETRS	SUNDlsMat_DenseGETRS

Table 1.1 – continued from previous page

Deprecated Name	New Name
denseGETRF	SUNDlsMat_denseGETRF
denseGETRS	SUNDlsMat_denseGETRS
DensePOTRF	SUNDlsMat_DensePOTRF
DensePOTRS	SUNDlsMat_DensePOTRS
densePOTRF	SUNDlsMat_densePOTRF
densePOTRS	SUNDlsMat_densePOTRS
DenseGEQRF	SUNDlsMat_DenseGEQRF
DenseORMQR	SUNDlsMat_DenseORMQR
denseGEQRF	SUNDlsMat_denseGEQRF
denseORMQR	SUNDlsMat_denseORMQR
DenseCopy	SUNDlsMat_DenseCopy
denseCopy	SUNDlsMat_denseCopy
DenseScale	SUNDlsMat_DenseScale
denseScale	SUNDlsMat_denseScale
denseAddIdentity	SUNDlsMat_denseAddIdentity
DenseMatvec	SUNDlsMat_DenseMatvec
denseMatvec	SUNDlsMat_denseMatvec
BandGBTRF	SUNDlsMat_BandGBTRF
bandGBTRF	SUNDlsMat_bandGBTRF
BandGBTRS	SUNDlsMat_BandGBTRS
bandGBTRS	SUNDlsMat_bandGBTRS
BandCopy	SUNDlsMat_BandCopy
bandCopy	SUNDlsMat_bandCopy
BandScale	SUNDlsMat_BandScale
bandScale	SUNDlsMat_bandScale
bandAddIdentity	SUNDlsMat_bandAddIdentity
BandMatvec	SUNDlsMat_BandMatvec
bandMatvec	SUNDlsMat_bandMatvec
ModifiedGS	SUNModifiedGS
ClassicalGS	SUNClassicalGS
QRfact	SUNQRFact
QRsol	SUNQRsol
DlsMat_NewDenseMat	SUNDlsMat_NewDenseMat
DlsMat_NewBandMat	SUNDlsMat_NewBandMat
DestroyMat	SUNDlsMat_DestroyMat
NewIntArray	SUNDlsMat_NewIntArray
NewIndexArray	SUNDlsMat_NewIndexArray
NewRealArray	SUNDlsMat_NewRealArray
DestroyArray	SUNDlsMat_DestroyArray
AddIdentity	SUNDlsMat_AddIdentity
SetToZero	SUNDlsMat_SetToZero
PrintMat	SUNDlsMat_PrintMat
newDenseMat	SUNDlsMat_newDenseMat
newBandMat	SUNDlsMat_newBandMat
destroyMat	SUNDlsMat_destroyMat
newIntArray	SUNDlsMat_newIntArray
newIndexArray	SUNDlsMat_newIndexArray
newRealArray	SUNDlsMat_newRealArray
destroyArray	SUNDlsMat_destroyArray

In addition, the entire sundials_lapack.h header file is now deprecated for removal in SUNDIALS v7.0.0. Note,

this header file is not needed to use the SUNDIALS LAPACK linear solvers.

1.2.14 Changes in v5.8.0

The *RAJA N_Vector* implementation has been updated to support the SYCL backend in addition to the CUDA and HIP backend. Users can choose the backend when configuring SUNDIALS by using the SUNDIALS_RAJA_BACKENDS CMake variable. This module remains experimental and is subject to change from version to version.

New *SUNMatrix* and *SUNLinearSolver* implementations were added to interface with the Intel oneAPI Math Kernel Library (oneMKL). Both the matrix and the linear solver support general dense linear systems as well as block diagonal linear systems. See §8.9 for more details. This module is experimental and is subject to change from version to version.

Added a new *optional* function to the SUNLinearSolver API, *SUNLinSolSetZeroGuess()*, to indicate that the next call to SUNlinSolSolve() will be made with a zero initial guess. SUNLinearSolver implementations that do not use the *SUNLinSolNewEmpty()* constructor will, at a minimum, need set the setzeroguess function pointer in the linear solver ops structure to NULL. The SUNDIALS iterative linear solver implementations have been updated to leverage this new set function to remove one dot product per solve.

CVODE now supports a new "matrix-embedded" *SUNLinearSolver* type. This type supports user-supplied *SUNLinearSolver* implementations that set up and solve the specified linear system at each linear solve call. Any matrix-related data structures are held internally to the linear solver itself, and are not provided by the SUNDIALS package.

Added specialized fused HIP kernels to CVODE which may offer better performance on smaller problems when using CVODE with the *N_Vector HIP* module. See the optional input function *CVodeSetUseIntegratorFusedKernels()* for more information. As with other SUNDIALS HIP features, this capability is considered experimental and may change from version to version.

Added the function *CVodeSetNlsRhsFn()* to supply an alternative right-hand side function for use within nonlinear system function evaluations.

The installed SUNDIALSConfig.cmake file now supports the COMPONENTS option to find_package. The exported targets no longer have IMPORTED_GLOBAL set.

A bug was fixed in *SUNMatCopyOps()* where the matrix-vector product setup function pointer was not copied.

A bug was fixed in the *SPBCGS* and *SPTFQMR* solvers for the case where a non-zero initial guess and a solution scaling vector are provided. This fix only impacts codes using *SPBCGS* or *SPTFQMR* as standalone solvers as all SUNDIALS packages utilize a zero initial guess.

1.2.15 Changes in v5.7.0

A new *N_Vector* implementation based on the SYCL abstraction layer has been added targeting Intel GPUs. At present the only SYCL compiler supported is the DPC++ (Intel oneAPI) compiler. See §6.12 for more details. This module is considered experimental and is subject to major changes even in minor releases.

New SUNMatrix and SUNLinearSolver implementations were added to interface with the MAGMA linear algebra library. Both the matrix and the linear solver support general dense linear systems as well as block diagonal linear systems, and both are targeted at GPUs (AMD or NVIDIA). See §8.8 for more details.

1.2.16 Changes in v5.6.1

Fixed a bug in the SUNDIALS CMake which caused an error if the `CMAKE_CXX_STANDARD` and `SUNDIALS_RAJA_-BACKENDS` options were not provided.

Fixed some compiler warnings when using the IBM XL compilers.

1.2.17 Changes in v5.6.0

A new *N_Vector* implementation based on the AMD ROCm HIP platform has been added. This vector can target NVIDIA or AMD GPUs. See §6.11 for more details. This module is considered experimental and is subject to change from version to version.

The *RAJA N_Vector* implementation has been updated to support the HIP backend in addition to the CUDA backend. Users can choose the backend when configuring SUNDIALS by using the `SUNDIALS_RAJA_BACKENDS` CMake variable. This module remains experimental and is subject to change from version to version.

A new optional operation, *N_VGetDeviceArrayPointer()*, was added to the N_Vector API. This operation is useful for N_Vectors that utilize dual memory spaces, e.g. the native SUNDIALS CUDA N_Vector.

The *SUNMATRIX_CUSPARSE* and *SUNLINEARSOLVER_CUSOLVERSP_BATCHQR* implementations no longer require the SUNDIALS *CUDA N_Vector*. Instead, they require that the vector utilized provides the *N_VGetDeviceArrayPointer()* operation, and that the pointer returned by *N_VGetDeviceArrayPointer()* is a valid CUDA device pointer.

1.2.18 Changes in v5.5.0

Refactored the SUNDIALS build system. CMake 3.12.0 or newer is now required. Users will likely see deprecation warnings, but otherwise the changes should be fully backwards compatible for almost all users. SUNDIALS now exports CMake targets and installs a SUNDIALSConfig.cmake file.

Added support for SuperLU DIST 6.3.0 or newer.

1.2.19 Changes in v5.4.0

Added new functions *CVodeComputeState()*, and *CVodeGetNonlinearSystemData()* which advanced users might find useful if providing a custom *SUNNonlinSolSysFn*.

Added the function *CVodeSetLSNormFactor()* to specify the factor for converting between integrator tolerances (WRMS norm) and linear solver tolerances (L2 norm) i.e., `tol_L2 = nrmfac * tol_WRMS`.

The expected behavior of *SUNNonlinSolGetNumIters()* and *SUNNonlinSolGetNumConvFails()* in the *SUNNonlinearSolver* API have been updated to specify that they should return the number of nonlinear solver iterations and convergence failures in the most recent solve respectively rather than the cumulative number of iterations and failures across all solves respectively. The API documentation and SUNDIALS provided *SUNNonlinearSolver* implementations have been updated accordingly. As before, the cumulative number of nonlinear iterations may be retreived by calling *CVodeGetNumNonlinSolvIters()*, the cumulative number of failures with *CVodeGetNumNonlinSolvConvFails()*, or both with *CVodeGetNonlinSolvStats()*.

A minor inconsistency in checking the Jacobian evaluation frequency has been fixed. As a result codes using using a non-default Jacobian update frequency through a call to CVodeSetMaxStepsBetweenJac() will need to increase the provided value by 1 to achieve the same behavior as before. For greater clarity the function has been deprecated and replaced with *CVodeSetJacEvalFrequency()*. Additionally, the function *CVodeSetLSetupFrequency()* has been added to set the frequency of calls to the linear solver setup function.

A new class, *SUNMemoryHelper*, was added to support **GPU users** who have complex memory management needs such as using memory pools. This is paired with new constructors for the `NVECTOR_CUDA` and `NVECTOR_RAJA` modules that accept a `SUNMemoryHelper` object. Refer to §4.6, §10, §6.10 and §6.13 for more information.

The `NVECTOR_RAJA` vector implementation has been updated to mirror the `NVECTOR_CUDA` implementation. Notably, the update adds managed memory support. Users of the vector will need to update any calls to the function because that signature was changed. This vector remains experimental and is subject to change from version to version.

The `NVECTOR_TRILINOS` vector implementation has been updated to work with Trilinos 12.18+. This update changes the local ordinal type to always be an `int`.

1.2.20 Changes in v5.3.0

Fixed a bug in the iterative linear solver modules where an error is not returned if the Atimes function is `NULL` or, if preconditioning is enabled, the PSolve function is `NULL`.

Added specialized fused CUDA kernels to CVODE which may offer better performance on smaller problems when using CVODE with the `NVECTOR_CUDA` module. See the optional input function for more information. As with other SUNDIALS CUDA features, this capability is considered experimental and may change from version to version.

Added the ability to control the CUDA kernel launch parameters for the `NVECTOR_CUDA` and `SUNMATRIX_CUSPARSE` modules. These modules remain experimental and are subject to change from version to version. In addition, the kernels were rewritten to be more flexible. Most users should see equivalent performance or some improvement, but a select few may observe minor performance degradation with the default settings. Users are encouraged to contact the SUNDIALS team about any perfomance changes that they notice.

Added new capabilities for monitoring the solve phase in the `SUNNONLINSOL_NEWTON` and `SUNNONLINSOL_FIXED-POINT` modules, and the SUNDIALS iterative linear solver modules. SUNDIALS must be built with the `SUNDIALS_-BUILD_WITH_MONITORING` CMake option set to `TRUE` to use these capabilties.

Added a new function, *CVodeSetMonitorFn()*, that takes a user-function to be called by CVODE after every nst succesfully completed time-steps. This is intended to provide a way of monitoring the CVODE statistics throughout the simulation.

Added a new function `CVodeGetLinSolveStats()` to get the CVODE linear solver statistics as a group.

Added the optional function `CVodeSetJacTimsRhsFn()` to specify an alternative right-hand side function for computing Jacobian-vector products with the internal difference quotient approximation.

Added support for integrating IVPs with constraints using BDF methods and projecting the solution onto the constraint manifold with a user defined projection function. This implementation is accompanied by additions to user documentation and CVODE examples. See *CVodeSetProjFn()* for more information.

Added support for CUDA v11.

1.2.21 Changes in v5.2.0

Fixed a build system bug related to the Fortran 2003 interfaces when using the IBM XL compiler. When building the Fortran 2003 interfaces with an XL compiler it is recommended to set `CMAKE_Fortran_COMPILER` to `f2003`, `xlf2003`, or `xlf2003_r`.

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

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

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

1.2.22 Changes in v5.1.0

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

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

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

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

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

Added support for constant damping to the *SUNNonlinearSolver_FixedPoint* module when using Anderson acceleration.

1.2.23 Changes in v5.0.0

Build system changes

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

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

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

NVECTOR module changes

- Two new functions were added to aid in creating custom `N_Vector` objects. The constructor *N_VNewEmpty()* allocates an "empty" generic `N_Vector` with the object's content pointer and the function pointers in the operations structure initialized to `NULL`. When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the `N_Vector` API by ensuring only required operations need to be set. Additionally, the function *N_VCopyOps()* has been added to copy the operation function pointers between vector objects. When used in clone routines for custom vector objects these functions also will ease the introduction of any new optional operations to the `N_Vector` API by ensuring all operations are copied when cloning objects. See §6.1.2 for more details.

- Two new `N_Vector` implementations, `NVECTOR_MANYVECTOR` and `NVECTOR_MPIMANYVECTOR`, have been created to support flexible partitioning of solution data among different processing elements (e.g., CPU + GPU) or for multi-physics problems that couple distinct MPI-based simulations together. This implementation is accompanied by additions to user documentation and SUNDIALS examples. See §6.17 and §6.18 for more details.

- One new required vector operation and ten new optional vector operations have been added to the `N_Vector` API. The new required operation, , returns the global length of an . The optional operations have been added to support the new `NVECTOR_MPIMANYVECTOR` implementation. The operation must be implemented by subvectors that are combined to create an `NVECTOR_MPIMANYVECTOR`, but is not used outside of this context. The remaining nine operations are optional local reduction operations intended to eliminate unnecessary latency when performing vector reduction operations (norms, etc.) on distributed memory systems. The optional local reduction vector operations are *N_VDotProdLocal()*, *N_VMaxNormLocal()*, *N_VL1NormLocal()*, *N_VWSqrSumLocal()*,

N_VWSqrSumMaskLocal(), *N_VInvTestLocal()*, *N_VConstrMaskLocal()*, *N_VMinLocal()*, and *N_VMin-QuotientLocal()*. If an `N_Vector` implementation defines any of the local operations as , then the NVECTOR_MPIMANYVECTOR will call standard `N_Vector` operations to complete the computation.

- An additional `N_Vector` implementation, NVECTOR_MPIPLUSX, has been created to support the MPI+X paradigm where X is a type of on-node parallelism (*e.g.*, OpenMP, CUDA). The implementation is accompanied by additions to user documentation and SUNDIALS examples. See §6.19 for more details.

- The and functions have been removed from the NVECTOR_CUDA and NVECTOR_RAJA implementations respectively. Accordingly, the `nvector_mpicuda.h`, `libsundials_nvecmpicuda.lib`, `libsundials_-nvecmpicudaraja.lib`, and files have been removed. Users should use the NVECTOR_MPIPLUSX module coupled in conjunction with the NVECTOR_CUDA or NVECTOR_RAJA modules to replace the functionality. The necessary changes are minimal and should require few code modifications. See the programs in and for examples of how to use the NVECTOR_MPIPLUSX module with the NVECTOR_CUDA and NVECTOR_RAJA modules respectively.

- Fixed a memory leak in the NVECTOR_PETSC module clone function.

- Made performance improvements to the NVECTOR_CUDA module. Users who utilize a non-default stream should no longer see default stream synchronizations after memory transfers.

- Added a new constructor to the NVECTOR_CUDA module that allows a user to provide custom allocate and free functions for the vector data array and internal reduction buffer. See §6.10 for more details.

- Added new Fortran 2003 interfaces for most `N_Vector` modules. See §6 for more details on how to use the interfaces.

- Added three new `N_Vector` utility functions *N_VGetVecAtIndexVectorArray()*, *N_VSetVecAtIndexVectorArray()*, and *N_VNewVectorArray()* for working with arrays when using the Fortran 2003 interfaces.

SUNMatrix module changes

- Two new functions were added to aid in creating custom `SUNMatrix` objects. The constructor *SUNMatNewEmpty()* allocates an "empty" generic `SUNMatrix` with the object's content pointer and the function pointers in the operations structure initialized to . When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the `SUNMatrix` API by ensuring only required operations need to be set. Additionally, the function *SUNMatCopyOps()* has been added to copy the operation function pointers between matrix objects. When used in clone routines for custom matrix objects these functions also will ease the introduction of any new optional operations to the `SUNMatrix` API by ensuring all operations are copied when cloning objects. See §7 for more details.

- A new operation, *SUNMatMatvecSetup()*, was added to the `SUNMatrix` API to perform any setup necessary for computing a matrix-vector product. This operation is useful for `SUNMatrix` implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product. Users who have implemented custom `SUNMatrix` modules will need to at least update their code to set the corresponding structure member to NULL. See §7.2 for more details.

- The generic `SUNMatrix` API now defines error codes to be returned by `SUNMatrix` operations. Operations which return an integer flag indiciating success/failure may return different values than previously. See §7.2.1 for more details.

- A new `SUNMatrix` (and `SUNLinearSolver`) implementation was added to facilitate the use of the SuperLU_-DIST library with SUNDIALS. See §7.9 for more details.

- Added new Fortran 2003 interfaces for most `SUNMatrix` modules. See §7 for more details on how to use the interfaces.

SUNLinearSolver module changes

- A new function was added to aid in creating custom `SUNLinearSolver` objects. The constructor allocates an "empty" generic `SUNLinearSolver` with the object's content pointer and the function pointers in the operations structure initialized to . When used in the constructor for custom objects this function will ease the introduction

of any new optional operations to the `SUNLinearSolver` API by ensuring only required operations need to be set. See §8.1.8 for more details.

- The return type of the `SUNLinearSolver` API function has changed from to to be consistent with the type used to store row indices in dense and banded linear solver modules.

- Added a new optional operation to the `SUNLinearSolver` API, *SUNLinSolLastFlag()*, that returns a for identifying the linear solver module.

- The `SUNLinearSolver` API has been updated to make the initialize and setup functions optional.

- A new `SUNLinearSolver` (and `SUNMatrix`) implementation was added to facilitate the use of the SuperLU_-DIST library with SUNDIALS. See §8.15 for more details.

- Added a new `SUNLinearSolver` implementation, *SUNLINEARSOLVER_CUSOLVERSP*, which leverages the NVIDIA cuSOLVER sparse batched QR method for efficiently solving block diagonal linear systems on NVIDIA GPUs.

- Added three new accessor functions to the SUNLINSOL_KLU module, *SUNLinSol_KLUGetSymbolic()*, , *SUN-LinSol_KLUGetNumeric()* and *SUNLinSol_KLUGetCommon()*, to provide user access to the underlying KLU solver structures. See §8.5 for more details.

- Added new Fortran 2003 interfaces for most `SUNLinearSolver` modules. See §8 for more details on how to use the interfaces.

SUNNonlinearSolver module changes

- A new function was added to aid in creating custom `SUNNonlinearSolver` objects. The constructor `SUN-NonlinSolSetConvTestFN()` allocates an "empty" generic `SUNNonlinearSolver` with the object's content pointer and the function pointers in the operations structure initialized to . When used in the constructor for custom objects this function will ease the introduction of any new optional operations to the `SUNNonlinearSolver` API by ensuring only required operations need to be set. See §9.1.7 for more details.

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

- The inputs values passed to the first two inputs of the function *SUNNonlinSolSolve()* in the `SUNNonlinearSolver` have been changed to be the predicted state and the initial guess for the correction to that state. Additionally, the definitions of *SUNNonlinSolLSetupFn()* and *SUNNonlinSolLSolveFn()* in the `SUNNonlinearSolver` API have been updated to remove unused input parameters. For more information on the nonlinear system formulation see §9.2 and for more details on the API functions see §9.

- Added a new `SUNNonlinearSolver` implementation, `SUNNONLINSOL_PETSC`, which interfaces to the PETSc SNES nonlinear solver API. See §9.5 for more details.

- Added new Fortran 2003 interfaces for most `SUNNonlinearSolver` modules. See §4.5 for more details on how to use the interfaces.

CVODE changes

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

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

- Fixed a memeory leak in FCVODE when not using the default nonlinear solver.

- Removed extraneous calls to for simulations where the scalar valued absolute tolerance, or all entries of the vector-valued absolute tolerance array, are strictly positive. In this scenario, CVODE will remove at least one global reduction per time step.

- The CVLS interface has been updated to only zero the Jacobian matrix before calling a user-supplied Jacobian evaluation function when the attached linear solver has type `SUNLINEARSOLVER_DIRECT`.

- A new linear solver interface function `CVLsLinSysFn()` was added as an alternative method for evaluating the linear system $M = I - \gamma J$.

- Added two new functions, `CVodeGetCurrentGamma()` and `CVodeGetCurrentState()`, which may be useful to users who choose to provide their own nonlinear solver implementations.

- The CVODE Fortran 2003 interface was completely redone to be more sustainable and to allow users to write more idiomatic Fortran. See §4.5 for more details.

1.2.24 Changes in v4.1.0

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

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

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

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

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

1.2.25 Changes in v4.0.2

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

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

1.2.26 Changes in v4.0.1

No changes were made in this release.

1.2.27 Changes in v4.0.0

CVODE's previous direct and iterative linear solver interfaces, CVDLS and CVSPILS, have been merged into a single unified linear solver interface, CVLS, to support any valid `SUNLinearSolver` module. This includes the "DIRECT" and "ITERATIVE" types as well as the new "MATRIX_ITERATIVE" type. Details regarding how CVLS utilizes linear solvers of each type as well as discussion regarding intended use cases for user-supplied `SUNLinearSolver` implementations are included in §8. All CVODE example programs and the standalone linear solver examples have been updated to use the unified linear solver interface.

The unified interface for the new CVLS module is very similar to the previous CVDLS and CVSPILS interfaces. To minimize challenges in user migration to the new names, the previous C and Fortran routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon. Additionally, we note that Fortran users, however, may need to enlarge their array of optional integer outputs, and update the indices that they query for certain linear-solver-related statistics.

The names of all constructor routines for SUNDIALS-provided `SUNLinearSolver` implementations have been updated to follow the naming convention `SUNLinSol_*` where is the name of the linear solver. Solver-specific "set"

routine names have been similarly standardized. To minimize challenges in user migration to the new names, the previous routine names may still be used; these will be deprecated in future releases, so we recommend that users migrate to the new names soon. All CVODE example programs and the standalone linear solver examples have been updated to use the new naming convention.

The *SUNMATRIX_BAND* constructor has been simplified to remove the storage upper bandwidth argument.

SUNDIALS integrators have been updated to utilize generic nonlinear solver modules defined through the SUNNonlinearSolver API. This API will ease the addition of new nonlinear solver options and allow for external or user-supplied nonlinear solvers. The SUNNonlinearSolver API and SUNDIALS provided modules are described in §9 and follow the same object oriented design and implementation used by the N_Vector, SUNMatrix, and SUNLinearSolver modules. Currently two SUNNonlinearSolver implementations are provided, SUNNONLINSOL_NEWTON and SUN-NONLINSOL_FIXEDPOINT. These replicate the previous integrator specific implementations of a Newton iteration and a fixed-point iteration (previously referred to as a functional iteration), respectively. Note the SUNNONLINSOL_FIXED-POINT module can optionally utilize Anderson's method to accelerate convergence. Example programs using each of these nonlinear solver modules in a standalone manner have been added and all CVODE example programs have been updated to use generic SUNNonlinearSolver modules.

With the introduction of SUNNonlinearSolver modules, the iter input parameter to *CVodeCreate()* has been removed along with the function CVodeSetIterType() and the constants CV_NEWTON and CV_FUNCTIONAL. Similarly, the parameter has been removed from the Fortran interface function FCVMALLOC. Instead of specifying the nonlinear iteration type when creating the CVODE memory structure, CVODE uses the SUNNONLINSOL_NEWTON module implementation of a Newton iteration by default. For details on using a non-default or user-supplied nonlinear solver see :numref:CVODE.Usage.CC. CVODE functions for setting the nonlinear solver options (e.g., *CVodeSetMaxNonlinIters()*) or getting nonlinear solver statistics (e.g., *CVodeGetNumNonlinSolvIters()*) remain unchanged and internally call generic SUNNonlinearSolver functions as needed.

Three fused vector operations and seven vector array operations have been added to the N_Vector API. These *optional* operations are disabled by default and may be activated by calling vector specific routines after creating an N_Vector (see §6 for more details). The new operations are intended to increase data reuse in vector operations, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. The fused operations are *N_VLinearCombination()*, *N_VScaleAddMulti()*, and *N_VDotProdMulti()* and the vector array operations are *N_VLinearCombinationVectorArray()*, *N_VScaleVectorArray()*, *N_VConstVectorArray()*, *N_VWrmsNormVectorArray()*, *N_VWrmsNormMaskVectorArray()*, and *N_VScaleAddMultiVectorArray()*. If an N_Vector implementation defines any of these operations as, then standard N_Vector operations will automatically be called as necessary to complete the computation.

Multiple updates to NVECTOR_CUDA were made:

- Changed to return the global vector length instead of the local vector length.

- Added to return the local vector length.

- Added to return the MPI communicator used.

- Removed the accessor functions in the namespace suncudavec.

- Changed the function to take a host data pointer and a device data pointer instead of an object.

- Added the ability to set the used for execution of the NVECTOR_CUDA kernels. See the function N_VSetCudaStream_Cuda().

- Added *N_VNewManaged_Cuda()*, *N_VMakeManaged_Cuda()*, and *N_VIsManagedMemory_Cuda()* functions to accommodate using managed memory with NVECTOR_CUDA.

Multiple changes to NVECTOR_RAJA were made:

- Changed to return the global vector length instead of the local vector length.

- Added to return the local vector length.

- Added to return the MPI communicator used.

- Removed the accessor functions in the namespace suncudavec.

- A new `N_Vector` implementation for leveraging OpenMP 4.5+ device offloading has been added, `NVECTOR_-OPENMPDEV`.

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

    - Fixed an efficiency bug where an extra call to the right hand side function was made.

    - Changed the behavior of the algorithm if the max-iterations case is hit. Before the algorithm would exit with the step size calculated on the penultimate iteration. Now it will exit with the step size calculated on the final iteration.

A Fortran 2003 interface to CVODE has been added along with Fortran 2003 interfaces to the following shared SUN-DIALS modules:

- `SUNNONLINSOL_FIXEDPOINT` and `SUNNONLINSOL_NEWTON` nonlinear solver modules

- `SUNLINSOL_BAND`, `SUNLINSOL_DENSE`, `SUNLINSOL_KLU`, `SUNLINSOL_PCG`, `SUNLINSOL_SPBCGS`, `SUNLIN-SOL_SPFGMR`, `SUNLINSOL_SPGMR`, and `SUNLINSOL_SPTFQMR` linear solver modules

- `NVECTOR_SERIAL`, `NVECTOR_PTHREADS`, and `NVECTOR_OPENMP` vector modules

1.2.28 Changes in v3.2.1

The changes in this minor release include the following:

- Fixed a bug in the CUDA `N_Vector` where the operation could write beyond the allocated vector data.

- Fixed library installation path for multiarch systems. This fix changes the default library installation path to `CMAKE_INSTALL_PREFIX/CMAKE_INSTALL_LIBDIR` from `CMAKE_INSTALL_PREFIX/lib`. `CMAKE_IN-STALL_LIBDIR` is automatically set, but is available as a CMake option that can modified.

1.2.29 Changes in v3.2.0

Support for optional inequality constraints on individual components of the solution vector has been added to CVODE and CVODES. See §2 and the description of in §5.5.10 for more details. Use of *CVodeSetConstraints()* requires the `N_Vector` operations *N_VMinQuotient()*, `N_VConstMask()`, and *N_VCompare()* that were not previously required by CVODE and CVODES.

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

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

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

Several changes were made to the build system:

- CMake 3.1.3 is now the minimum required CMake version.

- Deprecate the behavior of the CMake option and added the CMake option to select the integer size.

- The native CMake FindMPI module is now used to locate an MPI installation.

- If MPI is enabled and MPI compiler wrappers are not set, the build system will check if can compile MPI programs before trying to locate and use an MPI installation.

- The previous options for setting MPI compiler wrappers and the executable for running MPI programs have been have been depreated. The new options that align with those used in native CMake FindMPI module are `MPI_C_COMPILER`, `MPO_CXX_COMPILER`, `MPI_Fortran_COMPILER`, and `MPIEXEC_EXECUTABLE`.

- When a Fortran name-mangling scheme is needed (e.g., is) the build system will infer the scheme from the Fortran compiler. If a Fortran compiler is not available or the inferred or default scheme needs to be overridden, the advanced options and can be used to manually set the name-mangling scheme and bypass trying to infer the scheme.

- Parts of the main CMakeLists.txt file were moved to new files in the and directories to make the CMake configuration file structure more modular.

1.2.30 Changes in v3.1.2

The changes in this minor release include the following:

- Updated the minimum required version of CMake to 2.8.12 and enabled using rpath by default to locate shared libraries on OSX.

- Fixed Windows specific problem where was not correctly defined when using 64-bit integers for the SUNDIALS index type. On Windows `sunindextype` is now defined as the MSVC basic type `__int64`.

- Added sparse SUNMatrix "Reallocate" routine to allow specification of the nonzero storage.

- Updated the KLU SUNLinearSolver module to set constants for the two reinitialization types, and fixed a bug in the full reinitialization approach where the sparse SUNMatrix pointer would go out of scope on some architectures.

- Updated the "ScaleAdd" and "ScaleAddI" implementations in the sparse SUNMatrix module to more optimally handle the case where the target matrix contained sufficient storage for the sum, but had the wrong sparsity pattern. The sum now occurs in-place, by performing the sum backwards in the existing storage. However, it is still more efficient if the user-supplied Jacobian routine allocates storage for the sum $I + \gamma J$ manually (with zero entries if needed).

- Added the following examples from the usage notes page of the SUNDIALS website, and updated them to work with SUNDIALS 3.x:

  - `cvDisc_dns.c`, which demonstrates using CVODE with discontinuous solutions or RHS.

  - `cvRoberts_dns_negsol.c`, which illustrates the use of the RHS function return value to control unphysical negative concentrations.

- Changed the LICENSE install path to *instdir/icnlude/sundials*.

1.2.31 Changes in v3.1.1

The changes in this minor release include the following:

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

- Fixed a potential memory leak in the SPGMR and SPFGMR linear solvers: if "Initialize" was called multiple times then the solver memory was reallocated (without being freed).

- Updated KLU `SUNLinearSolver` module to use a for the precision-specific solve function to be used (to avoid compiler warnings).

- Added missing typecasts for some pointers (again, to avoid compiler warnings).

- Bugfix in `sunmatric_sparse.c` where we had used instead of in one location.

- Added missing `#include <stio.h>` in `N_Vector` and `SUNMatrix` header files.

- Fixed an indexing bug in the CUDA `N_Vector` implementation of and revised the RAJA `N_Vector` implementation of *N_VWrmsNormMask()* to work with mask arrays using values other than zero or one. Replaced `double` with `realtype` in the RAJA vector test functions.

- Fixed compilation issue with GCC 7.3.0 and Fortran programs that do not require a `SUNMatrix` or `SUNLinear-Solver` module (e.g., iterative linear solvers or fixed-point iteration).

In addition to the changes above, minor corrections were also made to the example programs, build system, and user documentation.

1.2.32 Changes in v3.1.0

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

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

1.2.33 Changes in v3.0.0

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

- Added generic SUNMATRIX module with three provided implementations: dense, banded and sparse. These replicate previous SUNDIALS Dls and Sls matrix structures in a single object-oriented API.

- Added example problems demonstrating use of generic SUNMATRIX modules.

- Added generic SUNLINEARSOLVER module with eleven provided implementations: dense, banded, LAPACK dense, LAPACK band, KLU, SuperLU_MT, SPGMR, SPBCGS, SPTFQMR, SPFGMR, PCG. These replicate previous SUNDIALS generic linear solvers in a single object-oriented API.

- Added example problems demonstrating use of generic SUNLINEARSOLVER modules.

- Expanded package-provided direct linear solver (Dls) interfaces and scaled, preconditioned, iterative linear solver (Spils) interfaces to utilize generic SUNMATRIX and SUNLINEARSOLVER objects.

- Removed package-specific, linear solver-specific, solver modules (e.g. CVDENSE, KINBAND, IDAKLU, ARK-SPGMR) since their functionality is entirely replicated by the generic Dls/Spils interfaces and SUNLINEAR-SOLVER/SUNMATRIX modules. The exception is CVDIAG, a diagonal approximate Jacobian solver available to CVODE and CVODES.

- Converted all SUNDIALS example problems to utilize new generic SUNMATRIX and SUNLINEARSOLVER objects, along with updated Dls and Spils linear solver interfaces.

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

Two additional `N_Vector` implementations were added – one for CUDA and one for RAJA vectors. These vectors are supplied to provide very basic support for running on GPU architectures. Users are advised that these vectors both move all data to the GPU device upon construction, and speedup will only be realized if the user also conducts the right-hand-side function evaluation on the device. In addition, these vectors assume the problem fits on one GPU. Further information about RAJA, users are referred to th web site, https://software.llnl.gov/RAJA/. These additions are accompanied by additions to various interface functions and to user documentation.

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

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

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

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

Added functions *SUNDIALSGetVersion()* and *SUNDIALSGetVersionNumber()* to get SUNDIALS release version information at runtime.

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

In addition, numerous changes were made to the build system. These include the addition of separate `BLAS_ENABLE` and `BLAS_LIBRARIES` CMake variables, additional error checking during CMake configuration, minor bug fixes, and renaming CMake options to enable/disable examples for greater clarity and an added option to enable/disable Fortran 77 examples. These changes included changing `EXAMPLES_ENABLE` to `EXAMPLES_ENABLE_C`, changing `CXX_ENABLE` to `EXAMPLES_ENABLE_CXX`, changing `F90_ENABLE` to `EXAMPLES_ENABLE_F90`, and adding an `EXAMPLES_ENABLE_F77` option.

A bug fix was made in *CVodeFree()* to call `lfree` unconditionally (if non-NULL).

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

1.2.34 Changes in v2.9.0

Two additional `N_Vector` 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 `N_Vector` module now includes a function, *N_VGetVectorID()*, that returns the `N_Vector` module name.

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

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

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

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

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

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

1.2.35 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 `N_Vector` 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 was ignored, and a line was added to break out of root-search loop if the initial interval size is below the tolerance `ttol`.

In `CVLapackBand`, the line `smu = MIN(N-1,mu+ml)` was changed to 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 to , and a few other names were also changed.

Two minor bugs were fixed regarding the testing of input on the first call to – one involving 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 were changed to `SUNMIN`, `SUNMAX`, `SUNSQR`, `SUNRabs`, `SUNRsqrt`, `SUNRexp`, `SUNRpowerI`, and `SUNRPowerR` respectively. These names occur in both the solver and in various example programs.

The example program `cvAdvDiff_diag_p` was added to illustrate the use of 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 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 `N_Vector` 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.

1.2.36 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 , 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 `CVSetTqBDF` each linear solver interface function, the linear solver memory is freed on an error return, and the 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 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.

1.2.37 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 -type function; and (c) a general streamlining of the preconditioner modules distributed with the solver.

1.2.38 Changes in v2.5.0

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

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.

1.2.39 Changes in v2.4.0

CVSPBCG and CVSPTFQMR modules have been added to interface with the Scaled Preconditioned Bi-CGstab (SP-BCG) and Scaled Preconditioned Transpose-Free Quasi-Minimal Residual (SPTFQMR) linear solver modules, respectively (for details see §5). 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 directory. For more details see §11.

1.2.40 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.

1.2.41 Changes in v2.2.1

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

1.2.42 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 and 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 - and -type routines. For more details see §5.5.10 and §5.5.12.

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 -type functions.

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

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

1.3 Reading this User Guide

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

There are different possible levels of usage of CVODE. The most casual user, with a small IVP problem only, can get by with reading §2.1, then §5 through §5.5.9 only, and looking at examples in [40].

In a different direction, a more expert user with an IVP problem may want to (a) use a package preconditioner (§5.7), (b) supply his/her own Jacobian or preconditioner routines (§5.6.7), (c) do multiple runs of problems of the same size (§5.5.13), (d) supply a new `N_Vector` module (§6), (e) supply new `SUNLinearSolver` and/or `SUNMatrix` modules (§7 and §8), or even (f) supply new `SUNNonlinearSolver` modules (§9).

The structure of this document is as follows:

- In §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 (§2.3), stability limit detection (§2.4), and rootfinding (§2.5).

- The following chapter describes the structure of the SUNDIALS suite of solvers (§3) and the software organization of the CVODE solver (§3.1).

- §5 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 §4.5, we describe the use of CVODE with Fortran applications.

- §6 gives a brief overview of the generic `N_Vector` module shared among the various components of SUNDIALS, and details on the `N_Vector` implementations provided with SUNDIALS.

- §7 gives a brief overview of the generic `SUNMatrix` module shared among the various components of SUNDIALS, and details on the `SUNMatrix` implementations provided with SUNDIALS: a dense implementation (§7.3), a banded implementation (§7.6) and a sparse implementation (§7.8).

- §8 gives a brief overview of the generic `SUNLinearSolver` module shared among the various components of SUNDIALS. This chapter contains details on the `SUNLinearSolver` implementations provided with SUNDIALS. The chapter also contains details on the `SUNLinearSolver` implementations provided with SUNDIALS that interface with external linear solver libraries.

- §9 describes the `SUNNonlinearSolver` API and nonlinear solver implementations shared among the various components of SUNDIALS.

- Finally, in the appendices, we provide detailed instructions for the installation of CVODE, within the structure of SUNDIALS (§11), as well as a list of all the constants used for input to and output from CVODE functions (§12).

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 are hyperlinked to their definitions directly; fields in C structures (such as *content*) appear in italics; and packages or modules, such as CVLS, are written in all capitals.

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1.4.3 SUNDIALS Release Numbers

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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

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

where $y \in \mathbb{R}^N$ and $f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$. Here we use $\dot{y}$ to denote $\mathrm{d}y/\mathrm{d}t$. 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.

For problems (2.1) where the analytical solution $y(t)$ satisfies an implicit constraint $g(t, y) = 0$ (including the initial condition, $g(t_0, y_0) = 0$) for $g(t, y) : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^M$ with $M < N$, CVODE may be configured to explicitly enforce these constraints via solving the modified problem

$$\begin{aligned} \dot{y} &= f(t, y), \quad y(t_0) = y_0, \\ 0 &= g(t, y). \end{aligned} \tag{2.2}$$

2.1 IVP solution

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

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

Here the y^n are computed approximations to $y(t_n)$, and $h_n = t_n - t_{n-1}$ is the step size. The user of CVODE must choose appropriately one of two multistep methods. For nonstiff problems, CVODE includes the Adams-Moulton formulas, characterized by $K_1 = 1$ and $K_2 = q - 1$ above, where the order q varies between 1 and 12. For stiff problems, CVODE includes the Backward Differentiation Formulas (BDF) in so-called fixed-leading coefficient (FLC) form, given by $K_1 = q$ and $K_2 = 0$, with order q varying between 1 and 5. The coefficients are uniquely determined by the method type, its order, the recent history of the step sizes, and the normalization $\alpha_{n,0} = -1$. See [18] and [41].

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

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

or as a fixed-point problem

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

where $a_n \equiv \sum_{i>0}(\alpha_{n,i}y^{n-i} + h_n\beta_{n,i}\dot{y}^{n-i})$.

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

$$W_i = 1/[\text{rtol} \cdot |y_i| + \text{atol}_i] \,. \tag{2.6}$$

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.

2.1.1 Nonlinear Solve

CVODE provides several nonlinear solver choices as well as the option of using a user-defined nonlinear solver (see §9). By default CVODE solves (2.4) with a *Newton iteration* which requires the solution of linear systems

$$M[y^{n(m+1)} - y^{n(m)}] = -F(y^{n(m)}) \,, \tag{2.7}$$

in which

$$M \approx I - \gamma J \,, \quad J = \partial f/\partial y \,, \quad \text{and} \quad \gamma = h_n\beta_{n,0} \,. \tag{2.8}$$

The exact variation of the Newton iteration depends on the choice of linear solver and is discussed below and in §9.3. For nonstiff systems, a *fixed-point iteration* (previously referred to as a functional iteration in this guide) solving (2.5) is also available. This involves evaluations of f only and can (optionally) use Anderson's method [9, 30, 47, 57] to accelerate convergence (see §9.4 for more details). For any nonlinear solver, the initial guess for the iteration is a predicted value $y^{n(0)}$ computed explicitly from the available history data.

For nonlinear solvers that require the solution of the linear system (2.7) (e.g., the default Newton iteration), CVODE provides several linear solver choices, including the option of a user-supplied linear solver module (see §8). The linear solver modules distributed with SUNDIALS are organized in two families, a *direct* family comprising direct linear solvers for dense, banded, or sparse matrices, and a *spils* family comprising scaled preconditioned iterative (Krylov) linear solvers. The methods offered through these modules are as follows:

- dense direct solvers, including an internal implementation, an interface to BLAS/LAPACK, an interface to MAGMA [53] and an interface to the oneMKL library [2],

- band direct solvers, including an internal implementation or an interface to BLAS/LAPACK,

- sparse direct solver interfaces to various libraries, including KLU [3, 23], SuperLU_MT [8, 25, 44], SuperLU_-Dist [7, 32, 45, 46], and cuSPARSE [6],

- SPGMR, a scaled preconditioned GMRES (Generalized Minimal Residual method) solver,

- SPFGMR, a scaled preconditioned FGMRES (Flexible Generalized Minimal Residual method) solver,

- SPBCG, a scaled preconditioned Bi-CGStab (Bi-Conjugate Gradient Stable method) solver,

- SPTFQMR, a scaled preconditioned TFQMR (Transpose-Free Quasi-Minimal Residual method) solver, or

- PCG, a scaled preconditioned CG (Conjugate Gradient method) solver.

For large stiff systems, where direct methods are often not feasible, the combination of a BDF integrator and a preconditioned Krylov method yields a powerful tool because it combines established methods for stiff integration, nonlinear iteration, and Krylov (linear) iteration with a problem-specific treatment of the dominant source of stiffness, in the form of the user-supplied preconditioner matrix [15].

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

In the case of a matrix-based linear solver, the default Newton iteration is a Modified Newton iteration, in that the iteration matrix M is fixed throughout the nonlinear iterations. However, in the case that a matrix-free iterative linear solver is used, the default Newton iteration is an Inexact Newton iteration, in which M is applied in a matrix-free manner, with matrix-vector products Jv obtained by either difference quotients or a user-supplied routine. With the default Newton iteration, the matrix M and preconditioner matrix P are updated as infrequently as possible to balance the high costs of matrix operations against other costs. Specifically, this matrix update occurs when:

- starting the problem,

- more than 20 steps have been taken since the last update,

- the value $\bar{\gamma}$ of γ at the last update satisfies $|\gamma/\bar{\gamma} - 1| > 0.3$,

- a non-fatal convergence failure just occurred, or

- an error test failure just occurred.

When an update of M or P occurs, it 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 update. Reevaluating J (or instructing the user to update Jacobian data in P) occurs when:

- starting the problem,

- more than 50 steps have been taken since the last evaluation,

- a convergence failure occurred with an outdated matrix, and the value $\bar{\gamma}$ of γ at the last update satisfies $|\gamma/\bar{\gamma} - 1| < 0.2$, or

- a convergence failure occurred that forced a step size reduction.

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

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

Now we use the estimate

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

Therefore the convergence (stopping) test is

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

We allow at most 3 iterations (but this limit can be changed by the user). We also declare the iteration diverged if any $\|\delta_m\|/\|\delta_{m-1}\| > 2$ with $m > 1$. If convergence fails with J or P current, we are forced to reduce the step size, and we replace h_n by $h_n = \eta_{\mathrm{cf}} * h_n$ where the default is $\eta_{\mathrm{cf}} = 0.25$. The integration is halted after a preset number of convergence failures; the default value of this limit is 10, but this can be changed by the user.

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

When the Jacobian is stored using either the *SUNMATRIX_DENSE* or *SUNMATRIX_BAND* matrix objects, the Jacobian may be supplied by a user routine, or approximated by difference quotients, at the user's option. In the latter case,

we use the usual approximation

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

The increments σ_j are given by

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

where U is the unit roundoff, σ_0 is a dimensionless value, and W_j is the error weight defined in (2.6). 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 sparse and user-supplied `SUNMatrix` objects, the Jacobian *must* be supplied by a user routine.

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

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

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

2.1.2 Local Error Test

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

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

2.1.3 Step Size and Order Selection

If the local error 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 $\eta = h'/h$ is limited above to $\eta_{\max\_ef}$ (default 0.2) after two error test failures, and limited below to $\eta_{\min\_ef}$ (default 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, 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

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

with q' set to the index achieving the above maximum. However, if we find that $\eta < \eta_{\text{max\_fx}}$ (default 1.5), we do not bother with the change. Also, η is always limited to $\eta_{\text{max\_gs}}$ (default 10), except on the first step, when it is limited to $\eta_{\text{max\_fs}} = 10^4$.

The various algorithmic features of CVODE described above, as inherited from VODE and VODPK, are documented in [14, 17, 37]. They are also summarized in [38].

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 $t = t_{\text{stop}}$.

2.1.4 Inequality Constraints

CVODE permits the user to impose optional inequality constraints on individual components of the solution vector y. Any of the following four constraints can be imposed: $y_i > 0$, $y_i < 0$, $y_i \geq 0$, or $y_i \leq 0$. The constraint satisfaction is tested after a successful nonlinear system solution. If any constraint fails, we declare a convergence failure of the Newton iteration and reduce the step size. Rather than cutting the step size by some arbitrary factor, CVODE estimates a new step size h' using a linear approximation of the components in y that failed the constraint test (including a safety factor of 0.9 to cover the strict inequality case). If a step fails to satisfy the constraints repeatedly within a step attempt or fails with the minimum step size then the integration is halted and an error is returned. In this case the user may need to employ other strategies as discussed in §5.5.2 to satisfy the inequality constraints.

2.2 IVPs with constraints

For IVPs whose analytical solutions implicitly satisfy constraints as in (2.2), CVODE ensures that the solution satisfies the constraint equation by projecting a successfully computed time step onto the invariant manifold. As discussed in [29] and [52], this approach reduces the error in the solution and retains the order of convergence of the numerical method. Therefore, in an attempt to advance the solution to a new point in time (i.e., taking a new integration step), CVODE performs the following operations:

1. predict solution

2. solve nonlinear system and correct solution

3. project solution

4. test error

5. select order and step size for next step

and includes several recovery attempts in case there are convergence failures (or difficulties) in the nonlinear solver or in the projection step, or if the solution fails to satisfy the error test. Note that at this time projection is only supported with BDF methods and the projection function must be user-defined. See §5.5.8 and *CVodeSetProjFn()* for more information on providing a projection function to CVODE.

When using a coordinate projection method the solution y_n is obtained by projecting (orthogonally or otherwise) the solution $\tilde{y}_n$ from step 2 above onto the manifold given by the constraint. As such y_n is computed as the solution of the nonlinear constrained least squares problem

$$
\begin{aligned}
\text{minimize} \quad & \|y_n - \tilde{y}_n\| \\
\text{subject to} \quad & g(t_n, y_n) = 0.
\end{aligned}
\tag{2.10}
$$

The solution of (2.10) can be computed iteratively with a Newton method. Given an initial guess $y_n^{(0)}$ the iterations are computed as

$$ y_n^{(i+1)} = y_n^{(i)} + \delta y_n^{(i)} $$

where the increment $\delta y_n^{(i)}$ is the solution of the least-norm problem

$$
\begin{aligned}
\text{minimize} \quad & \|\delta y_n^{(i)}\| \\
\text{subject to} \quad & G(t_n, y_n^{(i)})\, \delta y_n^{(i)} = -g(t_n, y_n^{(i)})
\end{aligned}
\tag{2.11}
$$

where $G(t, y) = \partial g(t, y)/\partial y$.

If the projected solution satisfies the error test then the step is accepted and the correction to the unprojected solution, $\Delta_p = y_n - \tilde{y}_n$, is used to update the Nordsieck history array for the next step.

2.3 Preconditioning

When using a nonlinear solver that requires the solution of the linear system, e.g., the default Newton iteration (§9.3), 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 supplied with SUNDIALS, these solvers are rarely successful if used without preconditioning; it is generally necessary to precondition the system in order to obtain acceptable efficiency. A system $Ax = b$ can be preconditioned on the left, as $(P^{-1}A)x = P^{-1}b$; on the right, as $(AP^{-1})Px = b$; or on both sides, as $(P_L^{-1}AP_R^{-1})P_Rx = P_L^{-1}b$. The Krylov method is then applied to a system with the matrix $P^{-1}A$, or AP^{-1}, or $P_L^{-1}AP_R^{-1}$, instead of A. In order to improve the convergence of the Krylov iteration, the preconditioner matrix P, or the product P_LP_R in the last case, should in some sense approximate the system matrix A. Yet at the same time, in order to be cost-effective, the matrix P, or matrices P_L and P_R, should be reasonably efficient to evaluate and solve. Finding a good point in this tradeoff between rapid convergence and low cost can be very difficult. Good choices are often problem-dependent (for example, see [15] for an extensive study of preconditioners for reaction-transport systems).

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

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

2.4 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 λ in the open left half-plane, the method is unconditionally stable (for any step size) for the standard scalar model problem $\dot{y} = \lambda y$. For an ODE system, this means that, roughly speaking, as long as all modes in the system are stable, the method is also stable for any choice of step size, at least in the sense of a local linear stability analysis.

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

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

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

The STALD algorithm attempts to detect, in a direct manner, the presence of a stability region boundary that is limiting the step sizes in the presence of a weakly damped oscillation [35]. The algorithm supplements (but differs greatly from) the existing algorithms in CVODE for choosing step size and order based on estimated local truncation errors. The STALD algorithm works directly with history data that is readily available in CVODE. If it concludes that the step size is in fact stability-limited, it dictates a reduction in the method order, regardless of the outcome of the error-based algorithm. The STALD algorithm has been tested in combination with the VODE solver on linear advection-dominated advection-diffusion problems [36], where it works well. The implementation in CVODE has been successfully tested on linear and nonlinear advection-diffusion problems, among others.

This stability limit detection option adds some computational overhead to the 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.

2.5 Rootfinding

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

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

The basic scheme used is to check for sign changes of any $g_i(t)$ over each time step taken, and then (when a sign change is found) to hone in on the root(s) with a modified secant method [34]. In addition, each time g is computed, CVODE checks to see if $g_i(t) = 0$ exactly, and if so it reports this as a root. However, if an exact zero of any g_i is found at a point t, CVODE computes g at $t + \delta$ for a small increment δ, slightly further in the direction of integration, and if any $g_i(t + \delta) = 0$ also, CVODE stops and reports an error. This way, each time CVODE takes a time step, it is guaranteed that the values of all g_i are nonzero at some past value of t, beyond which a search for roots is to be done.

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

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

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

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

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

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

Chapter 3

Code Organization

SUNDIALS consists of the solvers CVODE and ARKODE for ordinary differential equation (ODE) systems, IDA for differential-algebraic (DAE) systems, and KINSOL for nonlinear 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 following is a list summarizes the basic functionality of each SUNDIALS package:

- CVODE, a solver for stiff and nonstiff ODE systems $\dot{y} = f(t, y)$ based on Adams and BDF methods;

- CVODES, a solver for stiff and nonstiff ODE systems with sensitivity analysis capabilities;

- ARKODE, a solver for stiff, nonstiff, mixed stiff-nonstiff, and multirate ODE systems $M(t)\dot{y} = f_1(t, y) + f_2(t, y)$ based on Runge-Kutta methods;

- IDA, a solver for differential-algebraic systems $F(t, y, \dot{y}) = 0$ based on BDF methods;

- IDAS, a solver for differential-algebraic systems with sensitivity analysis capabilities;

- KINSOL, a solver for nonlinear algebraic systems $F(u) = 0$.

The various packages in the suite share many common components and are organized as a family. Fig. 3.1 gives a high-level overview of solver packages, the shared vector, matrix, linear solver, and nonlinear solver interfaces (abstract base classes), and the corresponding class implementations provided with SUNDIALS. For classes that provide interfaces to third-party libraries (i.e., LAPACK, KLU, SuperLU_MT, SuperLU_DIST, *hypre*, PETSc, Trilinos, and Raja) users will need to download and compile those packages independently of SUNDIALS. The directory structure is shown in Fig. 3.2.

3.1 CVODE organization

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

The overall organization of the CVODE package is shown in Figure Fig. 3.3.

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

CVODE utilizes generic linear and nonlinear solver modules defined by the `SUNLinearSolver` API (see §8) and `SUNNonlinearSolver` API (see §9) respectively. As such, CVODE has no knowledge of the method being used to solve the linear and nonlinear systems that arise. For any given user problem, there exists a single nonlinear solver
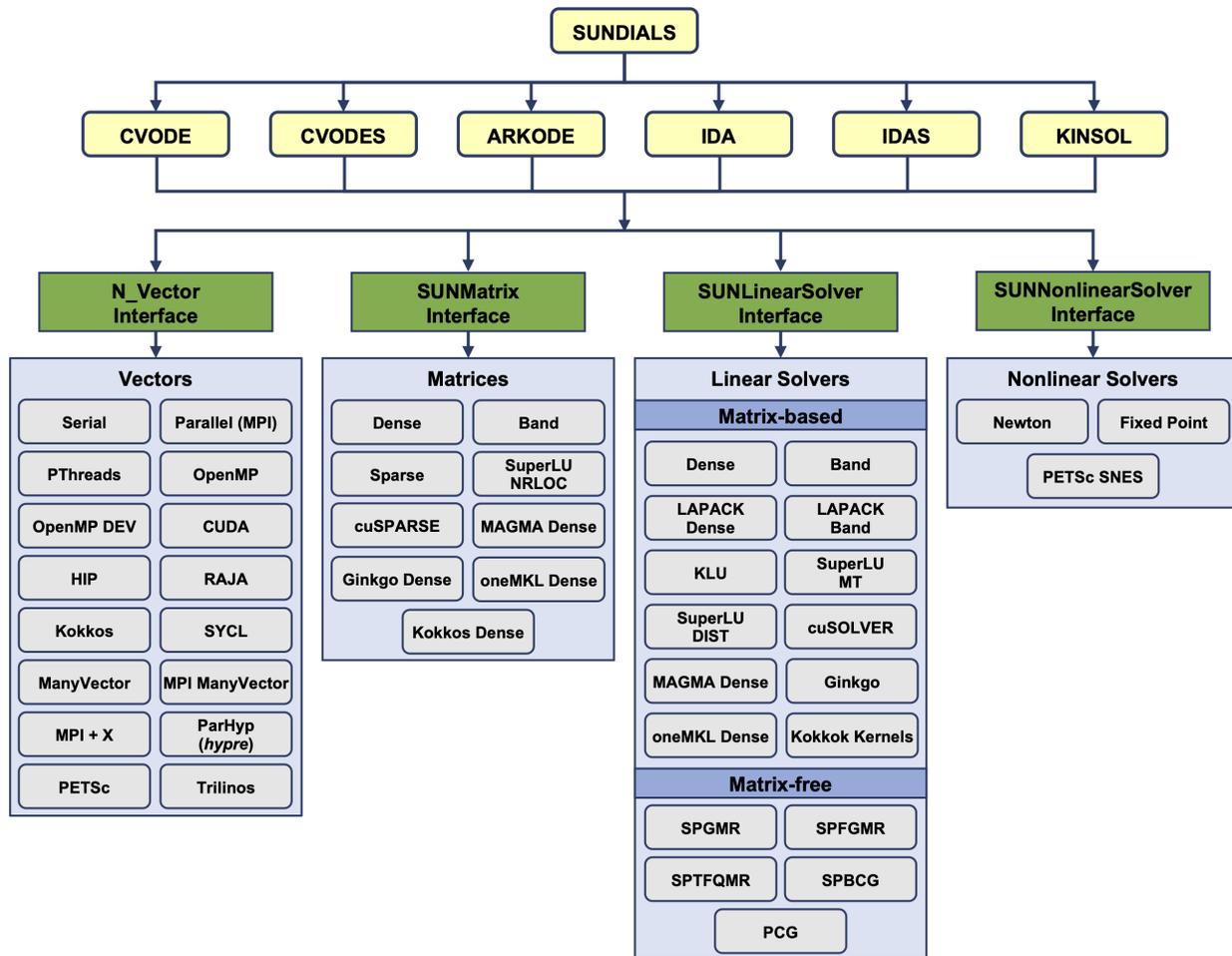
Fig. 3.1: High-level diagram of the SUNDIALS suite.
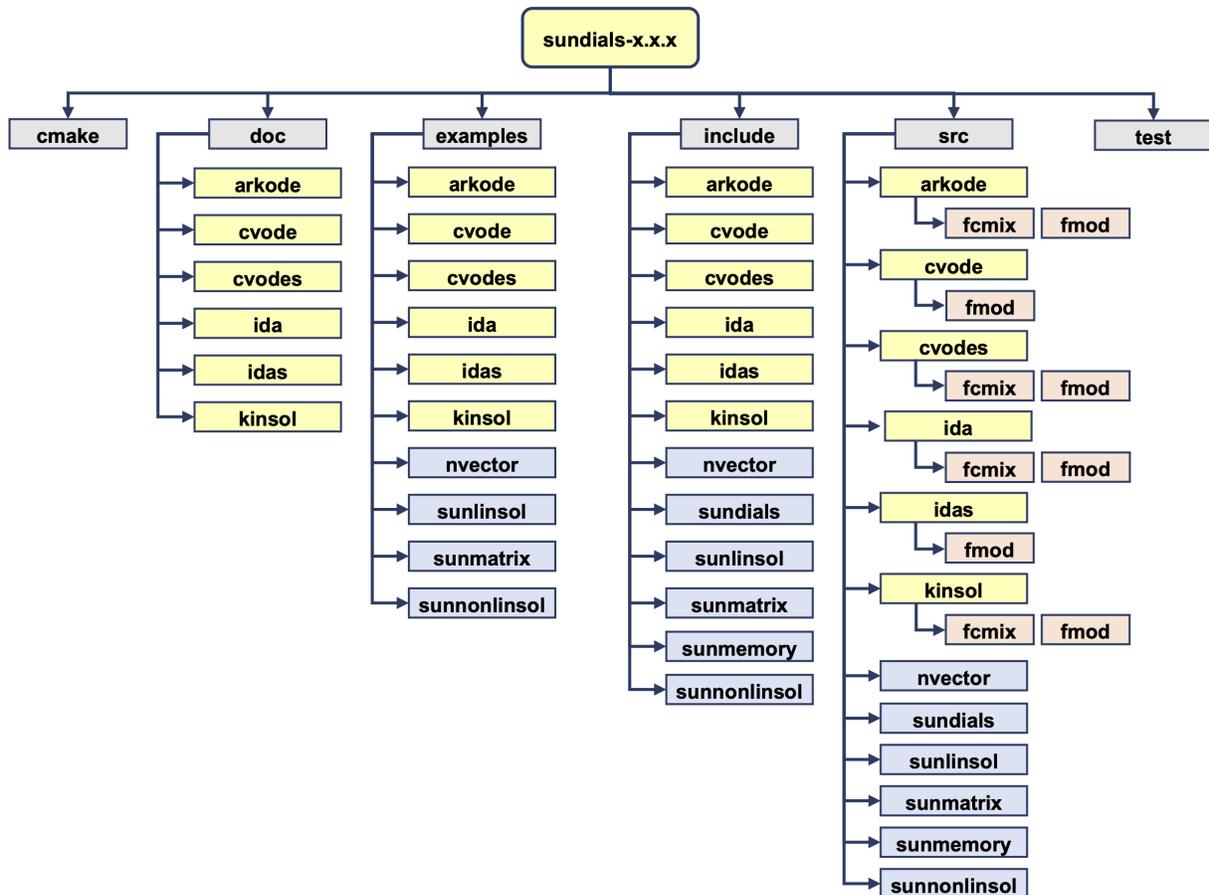
Fig. 3.2: Directory structure of the SUNDIALS source tree.
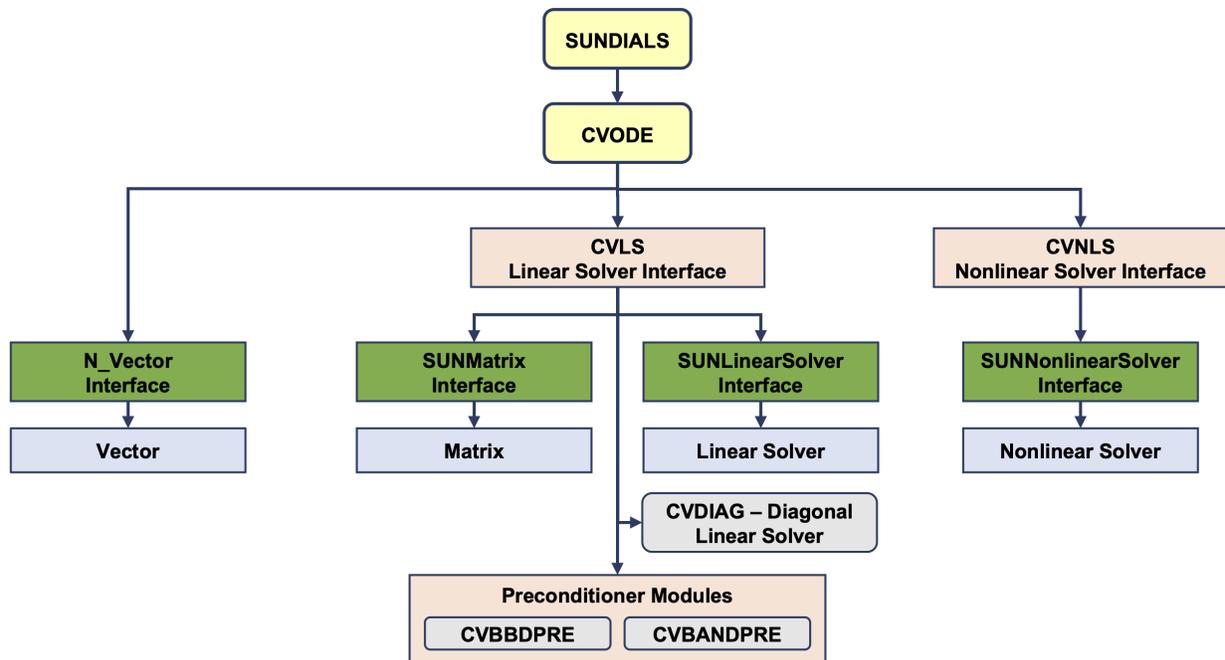
Fig. 3.3: Overall structure diagram of the CVODE package. Modules specific to CVODE begin with "CV" (CVLS, CVNLS, CVDIAG, CVBBDPRE, and CVBANDPRE), all other items correspond to generic SUNDIALS vector, matrix, and solver modules.

interface and, if necessary, one of the linear system solver interfaces is specified, and invoked as needed during the integration.

At present, the package includes two linear solver interfaces. The primary linear solver interface, CVLS, supports both direct and iterative linear solvers built using the generic `SUNLinearSolver` API (see §8). These solvers may utilize a `SUNMatrix` object (see §7) for storing Jacobian information, or they may be matrix-free. Since CVODE can operate on any valid `SUNLinearSolver` implementation, the set of linear solver modules available to CVODE will expand as new `SUNLinearSolver` modules are developed.

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

For users employing *SUNMATRIX_DENSE* or *SUNMATRIX_BAND* Jacobian matrices, CVODE includes algorithms for their approximation through difference quotients, although the user also has the option of supplying a routine to compute the Jacobian (or an approximation to it) directly. This user-supplied routine is required when using sparse or user-supplied Jacobian matrices.

For users employing matrix-free iterative linear solvers, CVODE includes an algorithm for the approximation by difference quotients of the product Mv. Again, the user has the option of providing routines for this operation, in two phases: setup (preprocessing of Jacobian data) and multiplication.

For preconditioned iterative methods, the preconditioning must be supplied by the user, again in two phases: setup and solve. While there is no default choice of preconditioner analogous to the difference-quotient approximation in the direct case, the references [15, 17], together with the example and demonstration programs included with CVODE, offer considerable assistance in building preconditioners.

CVODE's linear solver interface consists of four primary phases, devoted to (1) memory allocation and initialization, (2) setup of the matrix data involved, (3) solution of the system, and (4) freeing of memory. The setup and solution phases are separate because the evaluation of Jacobians and preconditioners is done only periodically during the integration, and only as required to achieve convergence.

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

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

Chapter 4

Using SUNDIALS

As discussed in §3, the six solvers packages (CVODE(S), IDA(S), ARKODE, KINSOL) that make up SUNDIALS are built upon common classes/modules for vectors, matrices, and algebraic solvers. In addition, the six packages all leverage some other common infrastructure, which we discuss in this section.

4.1 The SUNContext Type

New in version 6.0.0.

All of the SUNDIALS objects (vectors, linear and nonlinear solvers, matrices, etc.) that collectively form a SUNDIALS simulation, hold a reference to a common simulation context object defined by the *SUNContext* class.

The *SUNContext* class/type is defined in the header file sundials/sundials_context.h as

typedef struct _SUNContext ***SUNContext**

Users should create a *SUNContext* object prior to any other calls to SUNDIALS library functions by calling:

int **SUNContext_Create**(void *comm, *SUNContext* *ctx)

>   Creates a *SUNContext* object associated with the thread of execution. The data of the *SUNContext* class is private.

>   **Arguments:**

>   - comm – a pointer to the MPI communicator or NULL if not using MPI.

>   - ctx – [in,out] upon successful exit, a pointer to the newly created *SUNContext* object.

>   **Returns:**

>   - Will return < 0 if an error occurs, and zero otherwise.

The created *SUNContext* object should be provided to the constructor routines for different SUNDIALS classes/modules e.g.,

```
SUNContext sunctx;
void* package_mem;
N_Vector x;

SUNContext_Create(NULL, &sunctx);
```

```
package_mem = CVodeCreate(..., sunctx);
package_mem = IDACreate(..., sunctx);
package_mem = KINCreate(..., sunctx);
package_mem = ARKStepCreate(..., sunctx);

x = N_VNew_<SomeVector>(..., sunctx);
```

After all other SUNDIALS code, the *SUNContext* object should be freed with a call to:

int **SUNContext_Free**(*SUNContext* *ctx)

> Frees the *SUNContext* object.
>
> **Arguments:**
>
> > • ctx – pointer to a valid *SUNContext* object, NULL upon successful return.
>
> **Returns:**
>
> > • Will return < 0 if an error occurs, and zero otherwise.

> **Warning:** When MPI is being used, the *SUNContext_Free()* must be called prior to MPI_Finalize.

The *SUNContext* API further consists of the following functions:

int **SUNContext_GetProfiler**(*SUNContext* ctx, *SUNProfiler* *profiler)

> Gets the *SUNProfiler* object associated with the *SUNContext* object.
>
> **Arguments:**
>
> > • ctx – a valid *SUNContext* object.
> >
> > • profiler – [in,out] a pointer to the *SUNProfiler* object associated with this context; will be NULL if profiling is not enabled.
>
> **Returns:**
>
> > • Will return < 0 if an error occurs, and zero otherwise.

int **SUNContext_SetProfiler**(*SUNContext* ctx, *SUNProfiler* profiler)

> Sets the *SUNProfiler* object associated with the *SUNContext* object.
>
> **Arguments:**
>
> > • ctx – a valid *SUNContext* object.
> >
> > • profiler – a *SUNProfiler* object to associate with this context; this is ignored if profiling is not enabled.
>
> **Returns:**
>
> > • Will return < 0 if an error occurs, and zero otherwise.

int **SUNContext_SetLogger**(*SUNContext* ctx, *SUNLogger* logger)

> Sets the *SUNLogger* object associated with the *SUNContext* object.
>
> **Arguments:**
>
> > • ctx – a valid *SUNContext* object.
> >
> > • logger – a *SUNLogger* object to associate with this context; this is ignored if profiling is not enabled.

Returns:

- Will return < 0 if an error occurs, and zero otherwise.

New in version 6.2.0.

int **SUNContext_GetLogger**(*SUNContext* ctx, *SUNLogger* *logger)

Gets the *SUNLogger* object associated with the *SUNContext* object.

Arguments:

- `ctx` – a valid *SUNContext* object.

- `logger` – [in,out] a pointer to the *SUNLogger* object associated with this context; will be `NULL` if profiling is not enabled.

Returns:

- Will return < 0 if an error occurs, and zero otherwise.

New in version 6.2.0.

4.1.1 Implications for task-based programming and multi-threading

Applications that need to have *concurrently initialized* SUNDIALS simulations need to take care to understand the following:

#. A *SUNContext* object must only be associated with *one* SUNDIALS simulation (a solver object and its associated vectors etc.) at a time.

- Concurrently initialized is not the same as concurrently executing. Even if two SUNDIALS simulations execute sequentially, if both are initialized at the same time with the same *SUNContext*, behavior is undefined.

- It is OK to reuse a *SUNContext* object with another SUNDIALS simulation after the first simulation has completed and all of the simulation's associated objects (vectors, matrices, algebraic solvers, etc.) have been destroyed.

#. The creation and destruction of a *SUNContext* object is cheap, especially in comparison to the cost of creating/destroying a SUNDIALS solver object.

The following (incomplete) code examples demonstrate these points using CVODE as the example SUNDIALS package.

```
SUNContext sunctxs[num_threads];
int cvode_initialized[num_threads];
void* cvode_mem[num_threads];

// Create
for (int i = 0; i < num_threads; i++) {
   sunctxs[i] = SUNContext_Create(...);
   cvode_mem[i] = CVodeCreate(..., sunctxs[i]);
   cvode_initialized[i] = 0; // not yet initialized
   // set optional cvode inputs...
}

// Solve
#pragma omp parallel for
for (int i = 0; i < num_problems; i++) {
   int retval = 0;
```

(continues on next page)

```
   int tid = omp_get_thread_num();
   if (!cvode_initialized[tid]) {
      retval = CVodeInit(cvode_mem[tid], ...);
      cvode_initialized[tid] = 1;
   } else {
      retval = CVodeReInit(cvode_mem[tid], ...);
   }
   CVode(cvode_mem[i], ...);
}

// Destroy
for (int i = 0; i < num_threads; i++) {
   // get optional cvode outputs...
   CVodeFree(&cvode_mem[i]);
   SUNContext_Free(&sunctxs[i]);
}
```

Since each thread has its own unique CVODE and SUNContext object pair, there should be no thread-safety issues. Users should be sure that you apply the same idea to the other SUNDIALS objects needed as well (e.g. an `N_Vector`).

The variation of the above code example demonstrates another possible approach:

```
// Create, Solve, Destroy
#pragma omp parallel for
for (int i = 0; i < num_problems; i++) {
   int retval = 0;
   void* cvode_mem;
   SUNContext sunctx;

   sunctx = SUNContext_Create(...);
   cvode_mem = CVodeCreate(..., sunctx);
   retval = CVodeInit(cvode_mem, ...);

   // set optional cvode inputs...

   CVode(cvode_mem, ...);

   // get optional cvode outputs...

   CVodeFree(&cvode_mem);
   SUNContext_Free(&sunctx);
}
```

So long as the overhead of creating/destroying the CVODE object is small compared to the cost of solving the ODE, this approach is a fine alternative to the first approach since *SUNContext_Create()* and *SUNContext_Free()* are much cheaper than the CVODE create/free routines.

4.1.2 Convenience class for C++ Users

For C++ users a RAII safe class, `sundials::Context`, is provided:

```cpp
namespace sundials {

class Context : public sundials::ConvertibleTo<SUNContext>
{
public:
explicit Context(void* comm = nullptr)
{
   sunctx_ = std::make_unique<SUNContext>();
   SUNContext_Create(comm, sunctx_.get());
}

/* disallow copy, but allow move construction */
Context(const Context&) = delete;
Context(Context&&)      = default;

/* disallow copy, but allow move operators */
Context& operator=(const Context&) = delete;
Context& operator=(Context&&) = default;

SUNContext Convert() override
{
   return *sunctx_.get();
}
SUNContext Convert() const override
{
   return *sunctx_.get();
}
operator SUNContext() override
{
   return *sunctx_.get();
}
operator SUNContext() const override
{
   return *sunctx_.get();
}

~Context()
{
   if (sunctx_) SUNContext_Free(sunctx_.get());
}

private:
std::unique_ptr<SUNContext> sunctx_;
};

} // namespace sundials
```

4.2 SUNDIALS Status Logging

New in version 6.2.0.

SUNDIALS includes a built-in logging functionality which can be used to direct error messages, warning messages, informational output, and debugging output to specified files. This capability requires enabling both build-time and run-time options to ensure the best possible performance is achieved.

4.2.1 Enabling Logging

To enable logging, the CMake option *SUNDIALS_LOGGING_LEVEL* must be set to a value greater than 0 when configuring SUNDIALS. This option specifies the maximum desired output level. See the documentation entry for *SUN-DIALS_LOGGING_LEVEL* for the numeric values correspond to errors, warnings, info output, and debug output where errors < warnings < info output < debug output < extra debug output. If it is desired that the logger is MPI-aware, then the option *SUNDIALS_LOGGING_ENABLE_MPI* is set to TRUE. More details in regards to configuring SUNDIALS with CMake can be found in §11.

When SUNDIALS is built with logging enabled, then the default logger (stored in the *SUNContext* object) may be configured through environment variables without any changes to user code. The available environment variables are:

```
SUNLOGGER_ERROR_FILENAME
SUNLOGGER_WARNING_FILENAME
SUNLOGGER_INFO_FILENAME
SUNLOGGER_DEBUG_FILENAME
```

These environment variables may be set to a filename string. There are two special filenames: stdout and stderr. These two filenames will result in output going to the standard output file and standard error file. The different variables may all be set to the same file, or to distinct files, or some combination there of. To disable output for one of the streams, then do not set the environment variable, or set it to an empty string.

> **Warning:** A non-default logger should be created prior to any other SUNDIALS calls in order to capture all log events.

> **Note:** If *SUNDIALS_LOGGING_LEVEL* was set to 1 (corresponding to error-level output) at build-time, then setting the environment variable SUNLOGGER_INFO_FILENAME will do nothing.

> **Note:** Extra debugging output is turned on by setting *SUNDIALS_LOGGING_LEVEL* to 5. This extra output includes vector-values (so long as the *N_Vector* used supports printing).

4.2.2 Logger API

The central piece of the Logger API is the *SUNLogger* type:

typedef struct SUNLogger_ ***SUNLogger**

When SUNDIALS is built with logging enabled, a default logging object is stored in the *SUNContext* object and can be accessed with a call to *SUNContext_GetLogger()*.

The enumerated type *SUNLogLevel* is used by some of the logging functions to identify the output level or file.

enum **SUNLogLevel**

> The SUNDIALS logging level

enumerator **SUN_LOGLEVEL_ALL**

> Represents all output levels

enumerator **SUN_LOGLEVEL_NONE**

> Represents none of the output levels

enumerator **SUN_LOGLEVEL_ERROR**

> Represents error-level logging messages

enumerator **SUN_LOGLEVEL_WARNING**

> Represents warning-level logging messages

enumerator **SUN_LOGLEVEL_INFO**

> Represents info-level logging messages

enumerator **SUN_LOGLEVEL_DEBUG**

> Represents deubg-level logging messages

The *SUNLogger* class provides the following methods.

int **SUNLogger_Create**(void *comm, int output_rank, *SUNLogger* *logger)

> Creates a new *SUNLogger* object.
>
> **Arguments:**
>
> > - comm – a pointer to the MPI communicator if MPI is enabled, otherwise can be NULL.
> >
> > - output_rank – the MPI rank used for output (can be -1 to print to all ranks).
> >
> > - **logger – [in,out] On input this is a pointer to a**
> >   *SUNLogger*, on output it will point to a new *SUNLogger* instance.
>
> **Returns:**
>
> > - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_CreateFromEnv**(void *comm, *SUNLogger* *logger)

> Creates a new *SUNLogger* object and opens the output streams/files from the environment variables:
>
> ```
> SUNLOGGER_ERROR_FILENAME
> SUNLOGGER_WARNING_FILENAME
> SUNLOGGER_INFO_FILENAME
> SUNLOGGER_DEBUG_FILENAME
> ```
>
> **Arguments:**
>
> > - comm – a pointer to the MPI communicator if MPI is enabled, otherwise can be NULL.

- **logger** – **[in,out] On input this is a pointer to a**
  SUNLogger, on output it will point to a new *SUNLogger* instance.

  Returns:

    - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_SetErrorFilename**(*SUNLogger* logger, const char *error_filename)

  Sets the filename for error output.

  Arguments:

    - `logger` – a *SUNLogger* object.

    - `error_filename` – the name of the file to use for error output.

  Returns:

    - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_SetWarningFilename**(*SUNLogger* logger, const char *warning_filename)

  Sets the filename for warning output.

  Arguments:

    - `logger` – a *SUNLogger* object.

    - `warning_filename` – the name of the file to use for warning output.

  Returns:

    - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_SetInfoFilename**(*SUNLogger* logger, const char *info_filename)

  Sets the filename for info output.

  Arguments:

    - `logger` – a *SUNLogger* object.

    - `info_filename` – the name of the file to use for info output.

  Returns:

    - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_SetDebugFilename**(*SUNLogger* logger, const char *debug_filename)

  Sets the filename for debug output.

  Arguments:

    - `logger` – a *SUNLogger* object.

    - `debug_filename` – the name of the file to use for debug output.

  Returns:

    - Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_QueueMsg**(*SUNLogger* logger, *SUNLogLevel* lvl, const char *scope, const char *label, const char *msg_txt, ...)

  Queues a message to the output log level.

  Arguments:

    - `logger` – a *SUNLogger* object.

- `lvl` – the message log level (i.e. error, warning, info, debug).

- `scope` – the message scope (e.g. the function name).

- `label` – the message label.

- `msg_txt` – the message text itself.

- `...` – the format string arguments

Returns:

- Returns zero if successful, or non-zero if an error occurred.

> **Warning:** When compiling for ANSI C / C89 / C90 (and without compiler extensions), it is dangerous to pass any user input to this function because it falls back to using `sprintf` with a fixed buffer size.
>
> It is **highly recommended** to compile with C99 or newer if your compiler does not support `snprintf` through extensions.

int **SUNLogger_Flush**(*SUNLogger* logger, *SUNLogLevel* lvl)

Flush the message queue(s).

Arguments:

- `logger` – a *SUNLogger* object.

- `lvl` – the message log level (i.e. error, warning, info, debug or all).

Returns:

- Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_GetOutputRank**(*SUNLogger* logger, int *output_rank)

Get the output MPI rank for the logger.

Arguments:

- `logger` – a *SUNLogger* object.

- `output_rank` – [in,out] On input this is a pointer to an int, on output it points to the int holding the output rank.

Returns:

- Returns zero if successful, or non-zero if an error occurred.

int **SUNLogger_Destroy**(*SUNLogger* *logger)

Free the memory for the *SUNLogger* object.

Arguments:

- `logger` – a pointer to the *SUNLogger* object.

Returns:

- Returns zero if successful, or non-zero if an error occur.

4.2.3 Example Usage

As previously mentioned, if it is enabled at build time, there is a default *SUNLogger* attached to a *SUNContext* instance when it is created. This logger can be configured using the environment variables, e.g.,

```
SUNDIALS_INFO_FILENAME=stdout ./examples/cvode/serial/cvKrylovDemo_ls
```

SUNDIALS also includes several example codes that demonstrate how to use the logging interface via the C API.

```
examples/arkode/CXX_serial/ark_analytic_sys.cpp
examples/cvode/serial/cvAdvDiff_bnd.c
examples/cvode/parallel/cvAdvDiff_diag_p.c
examples/kinsol/CXX_parallel/kin_em_p.cpp
examples/kinsol/CUDA_mpi/kin_em_mpicuda.cpp
```

4.3 Performance Profiling

New in version 6.0.0.

SUNDIALS includes a lightweight performance profiling layer that can be enabled at compile-time. Optionally, this profiling layer can leverage Caliper [12] for more advanced instrumentation and profiling. By default, only SUNDIALS library code is profiled. However, a public profiling API can be utilized to leverage the SUNDIALS profiler to time user code regions as well (see §4.3.2).

4.3.1 Enabling Profiling

To enable profiling, SUNDIALS must be built with the CMake option *SUNDIALS_BUILD_WITH_PROFILING* set to ON. To utilize Caliper support, the CMake option *ENABLE_CALIPER* must also be set to ON. More details in regards to configuring SUNDIALS with CMake can be found in §11.

When SUNDIALS is built with profiling enabled and **without Caliper**, then the environment variable SUNPROFILER_-PRINT can be utilized to enable/disable the printing of profiler information. Setting SUNPROFILER_PRINT=1 will cause the profiling information to be printed to stdout when the SUNDIALS simulation context is freed. Setting SUNPRO-FILER_PRINT=0 will result in no profiling information being printed unless the *SUNProfiler_Print()* function is called explicitly. By default, SUNPROFILER_PRINT is assumed to be 0. SUNPROFILER_PRINT can also be set to a file path where the output should be printed.

If Caliper is enabled, then users should refer to the Caliper documentation for information on getting profiler output. In most cases, this involves setting the CALI_CONFIG environment variable.

Note: The SUNDIALS profiler requires POSIX timers or the Windows profileapi.h timers.

Warning: While the SUNDIALS profiling scheme is relatively lightweight, enabling profiling can still negatively impact performance. As such, it is recommended that profiling is enabled judiciously.

4.3.2 Profiler API

The primary way of interacting with the SUNDIALS profiler is through the following macros:

```
SUNDIALS_MARK_FUNCTION_BEGIN(profobj)
SUNDIALS_MARK_FUNCTION_END(profobj)
SUNDIALS_WRAP_STATEMENT(profobj, name, stmt)
SUNDIALS_MARK_BEGIN(profobj, name)
SUNDIALS_MARK_END(profobj, name)
```

Additionally, in C++ applications, the follow macro is available:

```
SUNDIALS_CXX_MARK_FUNCTION(profobj)
```

These macros can be used to time specific functions or code regions. When using the `*_BEGIN` macros, it is important that a matching `*_END` macro is placed at all exit points for the scope/function. The `SUNDIALS_CXX_MARK_FUNCTION` macro only needs to be placed at the beginning of a function, and leverages RAII to implicitly end the region.

The `profobj` argument to the macro should be a `SUNProfiler` object, i.e. an instance of the struct

typedef struct _SUNProfiler ***SUNProfiler**

When SUNDIALS is built with profiling, a default profiling object is stored in the `SUNContext` object and can be accessed with a call to *SUNContext_GetProfiler()*.

The `name` argument should be a unique string indicating the name of the region/function. It is important that the name given to the `*_BEGIN` macros matches the name given to the `*_END` macros.

In addition to the macros, the following methods of the `SUNProfiler` class are available.

int **SUNProfiler_Create**(void *comm, const char *title, *SUNProfiler* *p)

>   Creates a new `SUNProfiler` object.

>   **Arguments:**

>> - `comm` – a pointer to the MPI communicator if MPI is enabled, otherwise can be `NULL`

>> - `title` – a title or description of the profiler

>> - `p` – [in,out] On input this is a pointer to a `SUNProfiler`, on output it will point to a new `SUNProfiler` instance

>   **Returns:**

>> - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_Free**(*SUNProfiler* *p)

>   Frees a `SUNProfiler` object.

>   **Arguments:**

>> - `p` – [in,out] On input this is a pointer to a `SUNProfiler`, on output it will be `NULL`

>   **Returns:**

>> - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_Begin**(*SUNProfiler* p, const char *name)

>   Starts timing the region indicated by the `name`.

>   **Arguments:**

>> - `p` – a `SUNProfiler` object

- name – a name for the profiling region

    Returns:

    - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_End**(*SUNProfiler* p, const char *name)

Ends the timing of a region indicated by the name.

Arguments:

- p – a SUNProfiler object

- name – a name for the profiling region

    Returns:

    - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_GetElapsedTime**(*SUNProfiler* p, const char *name, double *time)

Get the elapsed time for the timer "name" in seconds.

Arguments:

- p – a SUNProfiler object

- name – the name for the profiling region of interest

- time – upon return, the elapsed time for the timer

    Returns:

    - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_GetTimerResolution**(*SUNProfiler* p, double *resolution)

Get the timer resolution in seconds.

Arguments:

- p – a SUNProfiler object

- resolution – upon return, the resolution for the timer

    Returns:

    - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_Print**(*SUNProfiler* p, FILE *fp)

Prints out a profiling summary. When constructed with an MPI comm the summary will include the average and maximum time per rank (in seconds) spent in each marked up region.

Arguments:

- p – a SUNProfiler object

- fp – the file handler to print to

    Returns:

    - Returns zero if successful, or non-zero if an error occurred

int **SUNProfiler_Reset**(*SUNProfiler* p)

Resets the region timings and counters to zero.

Arguments:

- p – a SUNProfiler object

Returns:

- Returns zero if successful, or non-zero if an error occurred

4.3.3 Example Usage

The following is an excerpt from the CVODE example code `examples/cvode/serial/cvAdvDiff_bnd.c`. It is applicable to any of the SUNDIALS solver packages.

```
SUNContext ctx;
SUNProfiler profobj;

/* Create the SUNDIALS context */
retval = SUNContext_Create(NULL, &ctx);

/* Get a reference to the profiler */
retval = SUNContext_GetProfiler(ctx, &profobj);

/* ... */

SUNDIALS_MARK_BEGIN(profobj, "Integration loop");
umax = N_VMaxNorm(u);
PrintHeader(reltol, abstol, umax);
for(iout=1, tout=T1; iout <= NOUT; iout++, tout += DTOUT) {
   retval = CVode(cvode_mem, tout, u, &t, CV_NORMAL);
   umax = N_VMaxNorm(u);
   retval = CVodeGetNumSteps(cvode_mem, &nst);
   PrintOutput(t, umax, nst);
}
SUNDIALS_MARK_END(profobj, "Integration loop");
PrintFinalStats(cvode_mem);  /* Print some final statistics   */
```

4.3.4 Other Considerations

If many regions are being timed, it may be necessary to increase the maximum number of profiler entries (the default is 2560). This can be done by setting the environment variable `SUNPROFILER_MAX_ENTRIES`.

4.4 SUNDIALS Version Information

SUNDIALS provides additional utilities to all packages, that may be used to retrieve SUNDIALS version information at runtime.

int **SUNDIALSGetVersion**(char *version, int len)

This routine fills a string with SUNDIALS version information.

Arguments:

- *version* – character array to hold the SUNDIALS version information.
- *len* – allocated length of the *version* character array.

Return value:

- 0 if successful

- -1 if the input string is too short to store the SUNDIALS version

Notes:

An array of 25 characters should be sufficient to hold the version information.

int **SUNDIALSGetVersionNumber**(int *major, int *minor, int *patch, char *label, int len)

This routine sets integers for the SUNDIALS major, minor, and patch release numbers and fills a string with the release label if applicable.

Arguments:

- *major* – SUNDIALS release major version number.

- *minor* – SUNDIALS release minor version number.

- *patch* – SUNDIALS release patch version number.

- *label* – string to hold the SUNDIALS release label.

- *len* – allocated length of the *label* character array.

Return value:

- 0 if successful

- -1 if the input string is too short to store the SUNDIALS label

Notes:

An array of 10 characters should be sufficient to hold the label information. If a label is not used in the release version, no information is copied to *label*.

4.5 SUNDIALS Fortran Interface

SUNDIALS provides modern, Fortran 2003 based, interfaces as Fortran modules to most of the C API including:

- All of the time-stepping modules in ARKODE:

    - The `farkode_arkstep_mod`, `farkode_erkstep_mod`, and `farkode_mristep_mod` modules provide interfaces to the ARKStep, ERKStep, and MRIStep integrators respectively.

    - The `farkode_mod` module interfaces to the components of ARKODE which are shared by the time-stepping modules.

- CVODE via the `fcvode_mod` module.

- CVODES via the `fcvodes_mod` module.

- IDA via the `fida_mod` module.

- IDAS via the `fidas_mod` module.

- KINSOL via the `fkinsol_mod` module.

Additionally, all of the SUNDIALS base classes (*N_Vector*, *SUNMatrix*, *SUNLinearSolver*, and *SUNNonlinear-Solver*) include Fortran interface modules. A complete list of class implementations with Fortran 2003 interface modules is given in Table 4.1.

An interface module can be accessed with the `use` statement, e.g.

```
use fcvode_mod
use fnvector_openmp_mod
```

and by linking to the Fortran 2003 library in addition to the C library, e.g. `libsundials_fnvecpenmp_mod.<so|a>`, `libsundials_nvecopenmp.<so|a>`, `libsundials_fcvode_mod.<so|a>` and `libsundials_cvode.<so|a>`.

The Fortran 2003 interfaces leverage the `iso_c_binding` module and the `bind(C)` attribute to closely follow the SUNDIALS C API (modulo language differences). The SUNDIALS classes, e.g. *N_Vector*, are interfaced as Fortran derived types, and function signatures are matched but with an `F` prepending the name, e.g. `FN_VConst` instead of *N_VConst()* or `FCVodeCreate` instead of `CVodeCreate`. Constants are named exactly as they are in the C API. Accordingly, using SUNDIALS via the Fortran 2003 interfaces looks just like using it in C. Some caveats stemming from the language differences are discussed in §4.5.2. A discussion on the topic of equivalent data types in C and Fortran 2003 is presented in §4.5.1.

Further information on the Fortran 2003 interfaces specific to the *N_Vector*, *SUNMatrix*, *SUNLinearSolver*, and *SUNNonlinearSolver* classes is given alongside the C documentation (§6, §7, §8, and §9 respectively). For details on where the Fortran 2003 module (`.mod`) files and libraries are installed see §11.

The Fortran 2003 interface modules were generated with SWIG Fortran [42], a fork of SWIG. Users who are interested in the SWIG code used in the generation process should contact the SUNDIALS development team.

Table 4.1: List of SUNDIALS Fortran 2003 interface modules

Class/Module	Fortran 2003 Module Name
ARKODE	`farkode_mod`
ARKODE::ARKSTEP	`farkode_arkstep_mod`
ARKODE::ERKSTEP	`farkode_erkstep_mod`
ARKODE::MRISTEP	`farkode_mristep_mod`
CVODE	`fcvode_mod`
CVODES	`fcvodes_mod`
IDA	`fida_mod`
IDAS	`fidas_mod`
KINSOL	`fkinsol_mod`
NVECTOR	`fsundials_nvector_mod`
NVECTOR_SERIAL	`fnvector_serial_mod`
NVECTOR_OPENMP	`fnvector_openmp_mod`
NVECTOR_PTHREADS	`fnvector_pthreads_mod`
NVECTOR_PARALLEL	`fnvector_parallel_mod`
NVECTOR_PARHYP	Not interfaced
NVECTOR_PETSC	Not interfaced
NVECTOR_CUDA	Not interfaced
NVECTOR_RAJA	Not interfaced
NVECTOR_SYCL	Not interfaced
NVECTOR_MANVECTOR	`fnvector_manyvector_mod`
NVECTOR_MPIMANVECTOR	`fnvector_mpimanyvector_mod`
NVECTOR_MPIPLUSX	`fnvector_mpiplusx_mod`
SUNMATRIX	`fsundials_matrix_mod`
SUNMATRIX_BAND	`fsunmatrix_band_mod`
SUNMATRIX_DENSE	`fsunmatrix_dense_mod`
SUNMATRIX_MAGMADENSE	Not interfaced
SUNMATRIX_ONEMKLDENSE	Not interfaced
SUNMATRIX_SPARSE	`fsunmatrix_sparse_mod`
SUNLINSOL	`fsundials_linearsolver_mod`
SUNLINSOL_BAND	`fsunlinsol_band_mod`
SUNLINSOL_DENSE	`fsunlinsol_dense_mod`
SUNLINSOL_LAPACKBAND	Not interfaced
SUNLINSOL_LAPACKDENSE	Not interfaced

Table 4.1 – continued from previous page

Class/Module	Fortran 2003 Module Name
SUNLINSOL_MAGMADENSE	Not interfaced
SUNLINSOL_ONEMKLDENSE	Not interfaced
SUNLINSOL_KLU	fsunlinsol_klu_mod
SUNLINSOL_SLUMT	Not interfaced
SUNLINSOL_SLUDIST	Not interfaced
SUNLINSOL_SPGMR	fsunlinsol_spgmr_mod
SUNLINSOL_SPFGMR	fsunlinsol_spfgmr_mod
SUNLINSOL_SPBCGS	fsunlinsol_spbcgs_mod
SUNLINSOL_SPTFQMR	fsunlinsol_sptfqmr_mod
SUNLINSOL_PCG	fsunlinsol_pcg_mof
SUNNONLINSOL	fsundials_nonlinearsolver_mod
SUNNONLINSOL_NEWTON	fsunnonlinsol_newton_mod
SUNNONLINSOL_FIXEDPOINT	fsunnonlinsol_fixedpoint_mod
SUNNONLINSOL_PETSCSNES	Not interfaced

4.5.1 Data Types

Generally, the Fortran 2003 type that is equivalent to the C type is what one would expect. Primitive types map to the `iso_c_binding` type equivalent. SUNDIALS classes map to a Fortran derived type. However, the handling of pointer types is not always clear as they can depend on the parameter direction. Table 4.2 presents a summary of the type equivalencies with the parameter direction in mind.

> **Warning:** Currently, the Fortran 2003 interfaces are only compatible with SUNDIALS builds where the `realtype` is double-precision the `sunindextype` size is 64-bits.

Table 4.2: C/Fortran-2003 Equivalent Types

C Type	Parameter Direction	Fortran 2003 type
double	in, inout, out, return	real(c_double)
int	in, inout, out, return	integer(c_int)
long	in, inout, out, return	integer(c_long)
booleantype	in, inout, out, return	integer(c_int)
realtype	in, inout, out, return	real(c_double)
sunindextype	in, inout, out, return	integer(c_long)
double*	in, inout, out	real(c_double), dimension(*)
double*	return	real(c_double), pointer, dimension(:)
int*	in, inout, out	real(c_int), dimension(*)
int*	return	real(c_int), pointer, dimension(:)
long*	in, inout, out	real(c_long), dimension(*)
long*	return	real(c_long), pointer, dimension(:)
realtype*	in, inout, out	real(c_double), dimension(*)
realtype*	return	real(c_double), pointer, dimension(:)
sunindextype*	in, inout, out	real(c_long), dimension(*)
sunindextype*	return	real(c_long), pointer, dimension(:)
realtype[]	in, inout, out	real(c_double), dimension(*)
sunindextype[]	in, inout, out	integer(c_long), dimension(*)
N_Vector	in, inout, out	type(N_Vector)

Table 4.2 – continued from previous page

C Type	Parameter Direction	Fortran 2003 type
N_Vector	return	type(N_Vector), pointer
SUNMatrix	in, inout, out	type(SUNMatrix)
SUNMatrix	return	type(SUNMatrix), pointer
SUNLinearSolver	in, inout, out	type(SUNLinearSolver)
SUNLinearSolver	return	type(SUNLinearSolver), pointer
SUNNonlinearSolver	in, inout, out	type(SUNNonlinearSolver)
SUNNonlinearSolver	return	type(SUNNonlinearSolver), pointer
FILE*	in, inout, out, return	type(c_ptr)
void*	in, inout, out, return	type(c_ptr)
T**	in, inout, out, return	type(c_ptr)
T***	in, inout, out, return	type(c_ptr)
T****	in, inout, out, return	type(c_ptr)

4.5.2 Notable Fortran/C usage differences

While the Fortran 2003 interface to SUNDIALS closely follows the C API, some differences are inevitable due to the differences between Fortran and C. In this section, we note the most critical differences. Additionally, §4.5.1 discusses equivalencies of data types in the two languages.

4.5.2.1 Creating generic SUNDIALS objects

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

C code:

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

Fortran code:

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

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

4.5.2.2 Arrays and pointers

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

C code:

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

/* create a new serial vector */
x = N_VNew_Serial(N, sunctx);

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

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

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

Fortran code:

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

! create a new serial vector
x => FN_VNew_Serial(x, sunctx)

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

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

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

4.5.2.3 Passing procedure pointers and user data

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

Typically when passing user data to a SUNDIALS function, a user may simply cast some custom data structure as a `void*`. When using the Fortran 2003 interfaces, the same thing can be achieved. Note, the custom data structure *does not* have to be `bind(C)` since it is never accessed on the C side.

C code:

```
MyUserData *udata;
void *cvode_mem;

ierr = CVodeSetUserData(cvode_mem, udata);
```

Fortran code:

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

ierr = FARKStepSetUserData(arkode_mem, c_loc(udata))
```

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

4.5.2.4 Passing `NULL` to optional parameters

In the SUNDIALS C API some functions have optional parameters that a caller can pass as NULL. If the optional parameter is of a type that is equivalent to a Fortran `type(c_ptr)` (see §4.5.1), then a Fortran user can pass the intrinsic `c_null_ptr`. However, if the optional parameter is of a type that is not equivalent to `type(c_ptr)`, then a caller must provide a Fortran pointer that is dissociated. This is demonstrated in the code example below.

C code:

```
SUNLinearSolver LS;
N_Vector x, b;

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

Fortran code:

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

! Disassociate A
A => null()

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

4.5.2.5 Working with `N_Vector` arrays

Arrays of `N_Vector` objects are interfaced to Fortran 2003 as an opaque `type(c_ptr)`. As such, it is not possible to directly index an array of `N_Vector` objects returned by the `N_Vector` "VectorArray" operations, or packages with sensitivity capabilities (CVODES and IDAS). Instead, SUNDIALS provides a utility function `FN_VGetVecAtIndexVectorArray()` that can be called for accessing a vector in a vector array. The example below demonstrates this:

C code:

```
N_Vector x;
N_Vector* vecs;

/* Create an array of N_Vectors */
vecs = N_VCloneVectorArray(count, x);
```

```c
/* Fill each array with ones */
for (int i = 0; i < count; ++i)
  N_VConst(vecs[i], 1.0);
```

Fortran code:

```fortran
type(N_Vector), pointer :: x, xi
type(c_ptr)             :: vecs

! Create an array of N_Vectors
vecs = FN_VCloneVectorArray(count, x)

! Fill each array with ones
do index = 0,count-1
  xi => FN_VGetVecAtIndexVectorArray(vecs, index)
  call FN_VConst(xi, 1.d0)
enddo
```

SUNDIALS also provides the functions *N_VSetVecAtIndexVectorArray()* and *N_VNewVectorArray()* for working with N_Vector arrays, that have corresponding Fortran interfaces FN_VSetVecAtIndexVectorArray and FN_-VNewVectorArray, respectively. These functions are particularly useful for users of the Fortran interface to the *NVECTOR_MANYVECTOR* or *NVECTOR_MPIMANYVECTOR* when creating the subvector array. Both of these functions along with *N_VGetVecAtIndexVectorArray()* (wrapped as FN_VGetVecAtIndexVectorArray) are further described in §6.1.1.

4.5.2.6 Providing file pointers

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

FILE *SUNDIALSFileOpen(filename, mode)

  The function allocates a FILE* by calling the C function fopen with the provided filename and I/O mode.

  Arguments:

  - filename – the path to the file, that should have Fortran type character(kind=C_CHAR, len=*). There are two special filenames: stdout and stderr – these two filenames will result in output going to the standard output file and standard error file, respectively.

  - mode – the I/O mode to use for the file. This should have the Fortran type character(kind=C_CHAR, len=*). The string begins with one of the following characters:

    – r to open a text file for reading

    – r+ to open a text file for reading/writing

    – w to truncate a text file to zero length or create it for writing

    – w+ to open a text file for reading/writing or create it if it does not exist

    – a to open a text file for appending, see documentation of fopen for your system/compiler

    – a+ to open a text file for reading/appending, see documentation for fopen for your system/compiler

  Return value:

  - The function returns a type(C_PTR) which holds a C FILE*.

void **SUNDIALSFileClose**(fp)

> The function deallocates a C FILE* by calling the C function `fclose` with the provided pointer.

> **Arguments:**

> > - `fp` – the C FILE* that was previously obtained from `fopen`. This should have the Fortran type `type(c_ptr)`. Note that if either `stdout` or `stderr` were opened using *SUNDIALSFileOpen()* then that stream *will not be closed* by this function.

4.5.3 Important notes on portability

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

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

4.5.4 Common Issues

In this subsection, we list some common issues users run into when using the Fortran interfaces.

Strange Segmentation Fault in User-Supplied Functions

One common issue we have seen trip up users (and even ourselves) has the symptom of segmentation fault in a user-supplied function (such as the RHS) when trying to use one of the callback arguments. For example, in the following RHS function, we will get a segfault on line 21:

```fortran
integer(c_int) function ff(t, yvec, ydotvec, user_data) &
   result(ierr) bind(C)

   use, intrinsic :: iso_c_binding
   use fsundials_nvector_mod
   implicit none

   real(c_double) :: t ! <===== Missing value attribute
   type(N_Vector) :: yvec
   type(N_Vector) :: ydotvec
   type(c_ptr)    :: user_data

   real(c_double) :: e
   real(c_double) :: u, v
   real(c_double) :: tmp1, tmp2
   real(c_double), pointer :: yarr(:)
   real(c_double), pointer :: ydotarr(:)

   ! get N_Vector data arrays
   yarr => FN_VGetArrayPointer(yvec)
   ydotarr => FN_VGetArrayPointer(ydotvec) ! <===== SEGFAULTS HERE

   ! extract variables
   u = yarr(1)
   v = yarr(2)
```

```
26
27    ! fill in the RHS function:
28    !  [0  0]*[(-1+u^2-r(t))/(2*u)] + [         0         ]
29    !  [e -1] [(-2+v^2-s(t))/(2*v)]    [sdot(t)/(2*vtrue(t))]
30    tmp1 = (-ONE+u*u-r(t))/(TWO*u)
31    tmp2 = (-TWO+v*v-s(t))/(TWO*v)
32    ydotarr(1) = ZERO
33    ydotarr(2) = e*tmp1 - tmp2 + sdot(t)/(TWO*vtrue(t))
34
35    ! return success
36    ierr = 0
37    return
38
39  end function
```

The subtle bug in the code causing the segfault is on line 8. It should read `real(c_double), value ::  t` instead of `real(c_double) ::  t` (notice the `value` attribute). Fundamental types that are passed by value in C need the `value` attribute.

4.6 Features for GPU Accelerated Computing

In this section, we introduce the SUNDIALS GPU programming model and highlight SUNDIALS GPU features. The model leverages the fact that all of the SUNDIALS packages interact with simulation data either through the shared vector, matrix, and solver APIs (see Chapters §6, §7, §8, and §9) or through user-supplied callback functions. Thus, under the model, the overall structure of the user's calling program, and the way users interact with the SUNDIALS packages is similar to using SUNDIALS in CPU-only environments.

4.6.1 SUNDIALS GPU Programming Model

As described in [11], within the SUNDIALS GPU programming model, all control logic executes on the CPU, and all simulation data resides wherever the vector or matrix object dictates as long as SUNDIALS is in control of the program. That is, SUNDIALS will not migrate data (explicitly) from one memory space to another. Except in the most advanced use cases, it is safe to assume that data is kept resident in the GPU-device memory space. The consequence of this is that, when control is passed from the user's calling program to SUNDIALS, simulation data in vector or matrix objects must be up-to-date in the device memory space. Similarly, when control is passed from SUNDIALS to the user's calling program, the user should assume that any simulation data in vector and matrix objects are up-to-date in the device memory space. To put it succinctly, *it is the responsibility of the user's calling program to manage data coherency between the CPU and GPU-device memory spaces* unless unified virtual memory (UVM), also known as managed memory, is being utilized. Typically, the GPU-enabled SUNDIALS modules provide functions to copy data from the host to the device and vice-versa as well as support for unmanaged memory or UVM. In practical terms, the way SUNDIALS handles distinct host and device memory spaces means that *users need to ensure that the user-supplied functions, e.g. the right-hand side function, only operate on simulation data in the device memory space* otherwise extra memory transfers will be required and performance will suffer. The exception to this rule is if some form of hybrid data partitioning (achievable with the NVECTOR_MANYVECTOR, see §6.17) is utilized.

SUNDIALS provides many native shared features and modules that are GPU-enabled. Currently, these include the NVIDIA CUDA platform [4], AMD ROCm/HIP [1], and Intel oneAPI [2]. Table 4.3–Table 4.6 summarize the shared SUNDIALS modules that are GPU-enabled, what GPU programming environments they support, and what class of memory they support (unmanaged or UVM). Users may also supply their own GPU-enabled `N_Vector`, `SUNMatrix`, `SUNLinearSolver`, or `SUNNonlinearSolver` implementation, and the capabilties will be leveraged since SUNDIALS operates on data through these APIs.

In addition, SUNDIALS provides a memory management helper module (see §10) to support applications which implement their own memory management or memory pooling.

Table 4.3: List of SUNDIALS GPU-enabled `N_Vector` Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
NVECTOR_CUDA	X			X	X
NVECTOR_HIP	X	X		X	X
NVECTOR_SYCL	X[3]	X[3]	X	X	X
NVECTOR_RAJA	X	X	X	X	X
NVECTOR_KOKKOS	X	X	X	X	X
NVECTOR_OPENMPDEV	X	X[2]	X[2]	X	

Table 4.4: List of SUNDIALS GPU-enabled `SUNMatrix` Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
SUNMATRIX_CUSPARSE	X			X	X
SUNMATRIX_ONEMKLDENSE	X[3]	X[3]	X	X	X
SUNMATRIX_MAGMADENSE	X	X		X	X
SUNMATRIX_GINKGO	X	X		X	X
SUNMATRIX_KOKKOSDENSE	X	X		X	X

Table 4.5: List of SUNDIALS GPU-enabled `SUNLinearSolver` Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
SUNLINSOL_CUSOLVERSP	X			X	X
SUNLINSOL_ONEMKLDENSE	X[3]	X[3]	X	X	X
SUNLINSOL_MAGMADENSE	X			X	X
SUNLINSOL_GINKGO	X	X		X	X
SUNLINSOL_KOKKOSDENSE	X	X		X	X
SUNLINSOL_SPGMR	X[1]	X[1]	X[1]	X[1]	X[1]
SUNLINSOL_SPFGMR	X[1]	X[1]	X[1]	X[1]	X[1]
SUNLINSOL_SPTFQMR	X[1]	X[1]	X[1]	X[1]	X[1]
SUNLINSOL_SPBCGS	X[1]	X[1]	X[1]	X[1]	X[1]
SUNLINSOL_PCG	X[1]	X[1]	X[1]	X[1]	X[1]

Table 4.6: List of SUNDIALS GPU-enabled `SUNNonlinearSolver` Modules

Module	CUDA	ROCm/HIP	oneAPI	Unmanaged Memory	UVM
SUNNONLINSOL_NEWTON	X[1]	X[1]	X[1]	X[1]	X[1]
SUNNONLINSOL_FIXEDPOINT	X[1]	X[1]	X[1]	X[1]	X[1]

Notes regarding the above tables:

1. This module inherits support from the NVECTOR module used

2. Support for ROCm/HIP and oneAPI are currently untested.

3. Support for CUDA and ROCm/HIP are currently untested.

In addition, note that implicit UVM (i.e. `malloc` returning UVM) is not accounted for.

4.6.2 Steps for Using GPU Accelerated SUNDIALS

For any SUNDIALS package, the generalized steps a user needs to take to use GPU accelerated SUNDIALS are:

1. Utilize a GPU-enabled `N_Vector` implementation. Initial data can be loaded on the host, but must be in the device memory space prior to handing control to SUNDIALS.

2. Utilize a GPU-enabled `SUNLinearSolver` linear solver (if applicable).

3. Utilize a GPU-enabled `SUNMatrix` implementation (if using a matrix-based linear solver).

4. Utilize a GPU-enabled `SUNNonlinearSolver` nonlinear solver (if applicable).

5. Write user-supplied functions so that they use data only in the device memory space (again, unless an atypical data partitioning is used). A few examples of these functions are the right-hand side evaluation function, the Jacobian evalution function, or the preconditioner evaulation function. In the context of CUDA and the right-hand side function, one way a user might ensure data is accessed on the device is, for example, calling a CUDA kernel, which does all of the computation, from a CPU function which simply extracts the underlying device data array from the `N_Vector` object that is passed from SUNDIALS to the user-supplied function.

Users should refer to the above tables for a complete list of GPU-enabled native SUNDIALS modules.

Chapter 5

Using CVODE for IVP Solution

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

The sample programs described in the companion document [40] may also be helpful. Those codes may be used as templates (with the removal of some lines used in testing) and are included in the CVODE package.

Users with applications written in Fortran should see §4.5, which describes interfacing with CVODE from Fortran.

The user should be aware that not all `SUNLinearSolver` and `SUNMatrix` modules are compatible with all `N_Vector` implementations. Details on compatibility are given in the documentation for each `SUNMatrix` module (§7) and each `SUNLinearSolver` module (§8). For example, `NVECTOR_PARALLEL` is not compatible with the dense, banded, or sparse `SUNMatrix` types, or with the corresponding dense, banded, or sparse `SUNLinearSolver` modules. Please check §7 and §8 to verify compatibility between these modules. In addition to that documentation, we note that the CVBANDPRE preconditioning module is only compatible with the `NVECTOR_SERIAL`, `NVECTOR_OPENMP`, and `NVECTOR_PTHREADS` vector implementations, and the preconditioner module CVBBDPRE can only be used with `NVECTOR_PARALLEL`. It is not recommended to use a threaded vector module with SuperLU_MT unless it is the `NVECTOR_OPENMP` module, and SuperLU_MT is also compiled with OpenMP.

CVODE uses various constants for both input and output. These are defined as needed in this chapter, but for convenience are also listed separately in §12.

5.1 Access to library and header files

At this point, it is assumed that the installation of CVODE, following the procedure described in §11, 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.<so|a>
<libdir>/libsundials_nvec*.<so|a>
<libdir>/libsundials_sunmat*.<so|a>
<libdir>/libsundials_sunlinsol*.<so|a>
<libdir>/libsundials_sunnonlinsol*.<so|a>
```

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

```
<incdir>/cvode
<incdir>/sundials
<incdir>/nvector
<incdir>/sunmatrix
<incdir>/sunlinsol
<incdir>/sunnonlinsol
```

The directories `libdir` and `incdir` are the install library and include directories, respectively. For a default installation, these are <instdir>/lib and <instdir>/include, respectively, where `instdir` is the directory where SUNDIALS was installed (§11).

5.2 Data Types

The header file `sundials_types.h` contains the definition of the types:

- *realtype* – the floating-point type used by the SUNDIALS packages

- *sunindextype* – the integer type used for vector and matrix indices

- *booleantype* – the type used for logic operations within SUNDIALS

- *SUNOutputFormat* – an enumerated type for SUNDIALS output formats

5.2.1 Floating point types

type **realtype**

The type `realtype` can be `float`, `double`, or `long double`, with the default being `double`. The user can change the precision of the arithmetic used in the SUNDIALS solvers at the configuration stage (see *SUNDIALS_- PRECISION*).

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 of `realtype`. In ANSI C, a floating-point constant with no suffix is stored as a `double`. Placing the suffix "F" at the end of a floating point constant makes it a `float`, whereas using the suffix "L" makes it a `long double`. For example,

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

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

Additionally, SUNDIALS defines several macros for common mathematical functions *e.g.*, `fabs`, `sqrt`, `exp`, etc. in `sundials_math.h`. The macros are prefixed with SUNR and expand to the appropriate C function based on the `realtype`. For example, the macro SUNRabs expands to the C function `fabs` when `realtype` is `double`, `fabsf` when `realtype` is `float`, and `fabsl` when `realtype` is `long double`.

A user program which uses the type `realtype`, the RCONST macro, and the SUNR mathematical function macros is precision-independent except for any calls to precision-specific library functions. Our example programs use `realtype`, RCONST, and the SUNR macros. Users can, however, use the type `double`, `float`, or `long double` in their code (assuming that this usage is consistent with the typedef for `realtype`) and call the appropriate math library functions directly. Thus, a previously existing piece of C or C++ code can use SUNDIALS without modifying the code to use `realtype`, RCONST, or the SUNR macros so long as the SUNDIALS libraries are built to use the corresponding precision (see §11.1.2).

5.2.2 Integer types used for indexing

type `sunindextype`

> The type `sunindextype` is used for indexing array entries in SUNDIALS modules as well as for storing the total problem size (*e.g.*, vector lengths and matrix sizes). During configuration `sunindextype` may be selected to be either a 32- or 64-bit *signed* integer with the default being 64-bit (see *SUNDIALS_INDEX_SIZE*).

When using a 32-bit integer the total problem size is limited to $2^{31} - 1$ and with 64-bit integers the limit is $2^{63} - 1$. For users with problem sizes that exceed the 64-bit limit an advanced configuration option is available to specify the type used for `sunindextype` (see *SUNDIALS_INDEX_TYPE*).

A user program which uses `sunindextype` to handle indices will work with both index storage types except for any calls to index storage-specific external libraries. Our C and C++ example programs use `sunindextype`. Users can, however, use any compatible type (*e.g.*, `int`, `long int`, `int32_t`, `int64_t`, or `long long int`) in their code, assuming that this usage is consistent with the typedef for `sunindextype` on their architecture. Thus, a previously existing piece of C or C++ code can use SUNDIALS without modifying the code to use `sunindextype`, so long as the SUNDIALS libraries use the appropriate index storage type (for details see §11.1.2).

5.2.3 Boolean type

type `booleantype`

> As ANSI C89 (ISO C90) does not have a built-in boolean data type, SUNDIALS defines the type `booleantype` as an `int`.

The advantage of using the name booleantype (instead of int) is an increase in code readability. It also allows the programmer to make a distinction between int and boolean data. Variables of type `booleantype` are intended to have only the two values SUNFALSE (`0`) and SUNTRUE (`1`).

5.2.4 Output formatting type

enum `SUNOutputFormat`

> The enumerated type *SUNOutputFormat* defines the enumeration constants for SUNDIALS output formats

enumerator `SUN_OUTPUTFORMAT_TABLE`

> The output will be a table of values

enumerator `SUN_OUTPUTFORMAT_CSV`

> The output will be a comma-separated list of key and value pairs e.g., `key1,value1,key2,value2,...`

Note: The file `scripts/sundials_csv.py` provides python utility functions to read and output the data from a SUNDIALS CSV output file using the key and value pair format.

5.3 Header files

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

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

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

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

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

If using a nonlinear solver that requires the solution of a linear system of the form (2.7) (e.g., the default Newton iteration), then a linear solver module header file will be required.

Other headers may be needed, according to the choice of preconditioner, etc. For example, in the example (see [40]), preconditioning is done with a block-diagonal matrix. For this, even though the `SUNLINSOL_SPGMR` linear solver is used, the header is included for access to the underlying generic dense matrix arithmetic routines.

5.4 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 `N_Vector`, `SUNMatrix`, `SUNLinearSolver`, and `SUNNonlinearSolver` implementations used. For the steps that are not, refer to §6, §7, §8, and §9 for the specific name of the function to be called or macro to be referenced.

1. **Initialize parallel or multi-threaded environment, if appropriate** For example, call `MPI_Init` to initialize MPI if used, or set the number of threads to use within the threaded vector functions if used.

2. **Create the SUNDIALS context object**
   Call *SUNContext_Create()* to allocate the `SUNContext` object.

3. **Set problem dimensions etc.** This generally includes the problem size `N`, and may include the local vector length `Nlocal`.

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

4. **Set vector of initial values** To set the vector of initial values, use the appropriate functions defined by the particular `N_Vector` implementation.

   For native SUNDIALS vector implementations, use a call of the form `y0 = N_VMake_***(..., ydata)` if the array containing the initial values of y already exists. Otherwise, create a new vector by making a call of the form `N_VNew_***(...)`, and then set its elements by accessing the underlying data with a call of the form `ydata = N_VGetArrayPointer(y0)`.

   For HYPRE and PETSC vector wrappers, first create and initialize the underlying vector, and then create an `N_Vector` wrapper with a call of the form `y0 = N_VMake_***(yvec)`, where `yvec` is a HYPRE or PETSC vector. Note that calls like `N_VNew_***(...)` and `N_VGetArrayPointer(...)` are not available for these vector wrappers.

   See §6 for details.

5. **Create CVODE object** Call `CVodeCreate()` to create the CVODE memory block and to specify the linear multistep method. `CVodeCreate()` returns a pointer to the CVODE memory structure.

    See §5.5.1 for details.

6. **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 §5.5.1 for details.

7. **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 §5.5.2 for details.

8. **Create matrix object** If a nonlinear solver requiring a linear solve will be used (e.g., the default Newton iteration) and the linear solver will be a matrix-based linear solver, then a template Jacobian matrix must be created by calling the appropriate constructor function defined by the particular `SUNMatrix` implementation.

    For the native SUNDIALS `SUNMatrix` implementations, the matrix object may be created using a call of the form `SUN***Matrix(...)` where `***` is the name of the matrix (see §7 for details).

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

    For any of the SUNDIALS-supplied `SUNLinearSolver` implementations, the linear solver object may be created using a call of the form `SUNLinearSolver LS = SUNLinSol_*(...)`; where `*` can be replaced with "Dense", "SPGMR", or other options, as discussed in §5.5.5 and §8.

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

11. **Attach linear solver module** If a nonlinear solver requiring a linear solver is chosen (e.g., the default Newton iteration), then initialize the CVLS linear solver interface by attaching the linear solver object (and matrix object, if applicable) with a call `ier = CVodeSetLinearSolver(cvode_mem, NLS)` (for details see §5.5.5):

    Alternately, if the CVODE-specific diagonal linear solver module, CVDIAG, is desired, initialize the linear solver module and attach it to CVODE with the call to `CVodeSetLinearSolver()`.

12. **Set optional inputs** Call `CVodeSet***` functions to change any optional inputs that control the behavior of CVODE from their default values. See §5.5.10 for details.

13. **Create nonlinear solver object** (*optional*) If using a non-default nonlinear solver (see §5.5.6), then create the desired nonlinear solver object by calling the appropriate constructor function defined by the particular `SUN-NonlinearSolver` implementation (e.g., `NLS = SUNNonlinSol_***(...)`; where `***` is the name of the nonlinear solver (see §9 for details).

14. **Attach nonlinear solver module** (*optional*) If using a non-default nonlinear solver, then initialize the nonlinear solver interface by attaching the nonlinear solver object by calling `ier = CVodeSetNonlinearSolver` (see §5.5.6 for details).

15. **Set nonlinear solver optional inputs** (*optional*) Call the appropriate set functions for the selected nonlinear solver module to change optional inputs specific to that nonlinear solver. These *must* be called after `CVodeInit()` if using the default nonlinear solver or after attaching a new nonlinear solver to CVODE, otherwise the optional inputs will be overridden by CVODE defaults. See §9 for more information on optional inputs.

16. **Specify rootfinding problem** (*optional*) Call `CVodeRootInit()` to initialize a rootfinding problem to be solved during the integration of the ODE system. See §5.5.7, and see §5.5.10.5 for relevant optional input calls.

---

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

18. **Get optional outputs** Call `CV*Get*` functions to obtain optional output. See §5.5.12 for details.

19. **Deallocate memory for solution vector** Upon completion of the integration, deallocate memory for the vector `y` (or `yout`) by calling the appropriate destructor function defined by the `N_Vector` implementation.

20. **Free solver memory** Call *CVodeFree()* to free the memory allocated by CVODE.

21. **Free nonlinear solver memory** (*optional*) If a non-default nonlinear solver was used, then call *SUNNonlinSol-Free()* to free any memory allocated for the `SUNNonlinearSolver` object.

22. **Free linear solver and matrix memory** Call *SUNLinSolFree()* and *SUNMatDestroy()* to free any memory allocated for the linear solver and matrix objects created above.

23. **Free the SUNContext object** Call *SUNContext_Free()* to free the memory allocated for the `SUNContext` object.

24. **Finalize MPI, if used** Call `MPI_Finalize` to terminate MPI.

5.5 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 §5.5.10, 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 §5.4 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 §5.5.10.1).

5.5.1 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.

void ***CVodeCreate**(int lmm, *SUNContext* sunctx)

> The function *CVodeCreate()* instantiates a CVODE solver object and specifies the solution method.
>
> **Arguments:**
>
> > - `lmm` – specifies the linear multistep method and must be one of two possible values: `CV_ADAMS` or `CV_BDF`.
> >
> > - `sunctx` – the *SUNContext* object (see §4.1)
>
> **Return Value:**
>
> > - If successful, *CVodeCreate()* returns a pointer to the newly created CVODE memory block (of type `void *`). Otherwise, it returns NULL.
>
> **Notes:** The recommended choices for `lmm` are `CV_ADAMS` for nonstiff problems and `CV_BDF` for stiff problems. The default Newton iteration is recommended for stiff problems, and the fixed-point solver (previously referred to as the functional iteration in this guide) is recommended for nonstiff problems. For details on how to attach a different nonlinear solver module to CVODE see the description of *CVodeSetNonlinearSolver()*.

int **CVodeInit**(void *cvode_mem, *CVRhsFn* f, *realtype* t0, *N_Vector* y0)

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

> **Arguments:**
>
> - `cvode_mem` – pointer to the CVODE memory block returned by *CVodeCreate()*.
>
> - `f` – is the C function which computes the right-hand side function f in the ODE. This function has the form `f(t, y, ydot, user_data)` (for full details see *CVRhsFn*).
>
> - `t0` – is the initial value of t.
>
> - `y0` – is the initial value of y.

> **Return Value:**
>
> - `CV_SUCCESS` – The call was successful.
>
> - `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> - `CV_MEM_FAIL` – A memory allocation request has failed.
>
> - `CV_ILL_INPUT` – An input argument to `CVodeInit` has an illegal value.

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

void **CVodeFree**(void **cvode_mem);

> The function `CVodeFree` frees the memory allocated by a previous call to *CVodeCreate()*.

> **Arguments:**
>
> - Pointer to the CVODE memory block.

> **Return Value:**
>
> - The function `CVodeFree` has no return value.

5.5.2 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()*

int **CVodeSStolerances**(void *cvode_mem, *realtype* reltol, *realtype* abstol)

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

> **Arguments:**
>
> - `cvode_mem` – pointer to the CVODE memory block returned by *CVodeCreate()*
>
> - `reltol` – is the scalar relative error tolerance.
>
> - `abstol` – is the scalar absolute error tolerance.

> **Return value:**
>
> - `CV_SUCCESS` – The call was successful
>
> - `CV_MEM_NULL` – The CVODE memory block was not initialized
>
> - `CV_NO_MALLOC` – The allocation function returned `NULL`
>
> - `CV_ILL_INPUT` – One of the input tolerances was negative.

int **CVodeSVtolerances**(void *cvode_mem, *realtype* reltol, *N_Vector* abstol)

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

>   **Arguments:**

>   - `cvode_mem` – pointer to the CVODE memory block returned by *CVodeCreate()*

>   - `reltol` – is the scalar relative error tolerance.

>   - `abstol` – is the vector of absolute error tolerances.

>   **Return value:**

>   - `CV_SUCCESS` – The call was successful

>   - `CV_MEM_NULL` – The CVODE memory block was not initialized

>   - `CV_NO_MALLOC` – The allocation function returned NULL

>   - `CV_ILL_INPUT` – The relative error tolerance was negative or the absolute tolerance had a negative component.

>   **Notes:**

>   This choice of tolerances is important when the absolute error tolerance needs to be different for each component of the state vector y.

int **CVodeWFtolerances**(void *cvode_mem, *CVEwtFn* efun)

>   The function `CVodeWFtolerances` specifies a user-supplied function `efun` that sets the multiplicative error weights W_i for use in the weighted RMS norm, which are normally defined by (2.6).

>   **Arguments:**

>   - `cvode_mem` – pointer to the CVODE memory block returned by *CVodeCreate()*

>   - `efun` – is the C function which defines the `ewt` vector (see *CVEwtFn*).

>   **Return value:**

>   - `CV_SUCCESS` – The call was successful

>   - `CV_MEM_NULL` – The CVODE memory block was not initialized

>   - `CV_NO_MALLOC` – The allocation function returned NULL

5.5.3 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 10^{-15}).

(2) The absolute tolerances `abstol` (whether scalar or vector) need to be set to control absolute errors when any components of the solution vector y may be so small that pure relative error control is meaningless. For example, if `y[i]` starts at some nonzero value, but in time decays to zero, then pure relative error control on `y[i]` makes no sense (and is overly costly) after `y[i]` is below some noise level. Then `abstol` (if scalar) or `abstol[i]` (if a vector) needs to be set to that noise level. If the different components have different noise levels, then `abstol` should be a vector. See the example `cvsRoberts_dns` in the CVODE package, and the discussion of it in the CVODE Examples document [51]. In that problem, the three components vary betwen 0 and 1, and have different noise levels; hence the `abstol` vector. It is impossible to give any general advice on `abstol` values, because the appropriate noise levels are completely problem-dependent. The user or modeler hopefully has some idea as to what those noise levels are.

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

5.5.4 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.

5.5.5 Linear solver interface functions

As previously explained, if the nonlinear solver requires the solution of linear systems of the form (2.7) (e.g., the default Newton iteration), there are two CVODE linear solver interfaces currently available for this task: CVLS and CVDIAG.

The first corresponds to the main linear solver interface in CVODE, that supports all valid `SUNLinearSolver` modules. Here, matrix-based `SUNLinearSolver` modules utilize `SUNMatrix` objects to store the approximate Jacobian matrix $J = \partial f / \partial y$, the Newton matrix $M = I - \gamma J$, and factorizations used throughout the solution process. Conversely, matrix-free `SUNLinearSolver` modules instead use iterative methods to solve the Newton systems of equations, and only require the *action* of the matrix on a vector, Mv. With most of these methods, preconditioning can be done on the left only, the right only, on both the left and right, or not at all. The exceptions to this rule are SPFGMR that supports right preconditioning only and PCG that performs symmetric preconditioning. For the specification of a preconditioner, see the iterative linear solver sections in §5.5.10 and §5.6.

If preconditioning is done, user-supplied functions define linear operators corresponding to left and right preconditioner matrices P_1 and P_2 (either of which could be the identity matrix), such that the product $P_1 P_2$ approximates the matrix $M = I - \gamma J$ of (2.8).

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

To specify a generic linear solver to CVODE, after the call to *CVodeCreate()* but before any calls to *CVode()*, the user's program must create the appropriate *SUNLinearSolver* object and call the function *CVodeSetLinear-Solver()*, as documented below. To create the *SUNLinearSolver* object, the user may call one of the SUNDIALS-packaged `SUNLinearSolver` module constructor routines via a call of the form `SUNLinearSolver LS = SUNLinSol_*(...);`

Alternately, a user-supplied *SUNLinearSolver* module may be created and used instead. The use of each of the generic linear solvers involves certain constants, functions and possibly some macros, that are likely to be needed in the user code. These are available in the corresponding header file associated with the specific SUNMatrix or SUNLinearSolver module in question, as described in §7 and §8.

Once this solver object has been constructed, the user should attach it to CVODE via a call to *CVodeSetLinearSolver()*. The first argument passed to this function is the CVODE memory pointer returned by *CVodeCreate()*; the second argument is the desired SUNLinearSolver object to use for solving linear systems. The third argument is an optional SUNMatrix object to accompany matrix-based SUNLinearSolver inputs (for matrix-free linear solvers, the third argument should be NULL). A call to this function initializes the CVLS linear solver interface, linking it to the main CVODE integrator, and allows the user to specify additional parameters and routines pertinent to their choice of linear solver.

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

int **CVodeSetLinearSolver**(void *cvode_mem, *SUNLinearSolver* LS, *SUNMatrix* J)

> The function CVodeSetLinearSolver attaches a generic SUNLinearSolver object LS and corresponding template Jacobian SUNMatrix object J (if applicable) to CVODE, initializing the CVLS linear solver interface.
>
> **Arguments:**
>> - cvode_mem – pointer to the CVODE memory block.
>> - LS – SUNLinearSolver object to use for solving linear systems of the form (2.7)
>> - J – SUNMatrix object for used as a template for the Jacobian (or NULL if not applicable).
>
> **Return value:**
>> - CVLS_SUCCESS – The CVLS initialization was successful.
>> - CVLS_MEM_NULL – The cvode_mem pointer is NULL.
>> - CVLS_ILL_INPUT – The CVLS interface is not compatible with the LS or J input objects or is incompatible with the current N_Vector module.
>> - CVLS_SUNLS_FAIL – A call to the LS object failed.
>> - CVLS_MEM_FAIL – A memory allocation request failed.
>
> **Notes:**
>> If LS is a matrix-based linear solver, then the template Jacobian matrix J will be used in the solve process, so if additional storage is required within the SUNMatrix object (e.g. for factorization of a banded matrix), ensure that the input object is allocated with sufficient size (see §7 for further information).
>>
>> When using sparse linear solvers, it is typically much more efficient to supply J so that it includes the full sparsity pattern of the Newton system matrices $M = I - \gamma J$, even if J itself has zeros in nonzero locations of I. The reasoning for this is that M is constructed in-place, on top of the user-specified values of J, so if the sparsity pattern in J is insufficient to store M then it will need to be resized internally by CVODE.
>>
>> The previous routines CVDlsSetLinearSolver and CVSpilsSetLinearSolver are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

int **CVDiag**(void *cvode_mem)

> The function CVDiag selects the CVDIAG linear solver. The user's main program must include the cvode_diag.h header file.
>
> **Arguments:**
>> - cvode_mem – pointer to the CVODE memory block.

Return value:

- `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 `N_Vector` module.

- `CVDIAG_MEM_FAIL` – A memory allocation request failed.

Notes:

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

5.5.6 Nonlinear solver interface function

By default CVODE uses the `SUNNonlinearSolver` implementation of Newton's method defined by the *SUNNON-LINSOL_NEWTON* module. To specify a different nonlinear solver in CVODE, the user's program must create a `SUNNonlinearSolver` object by calling the appropriate constructor routine. The user must then attach the `SUNNonlinearSolver` object by calling *CVodeSetNonlinearSolver()*, as documented below.

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

The first argument passed to the routine *CVodeSetNonlinearSolver()* is the CVODE memory pointer returned by *CVodeCreate()* and the second argument is the `SUNNonlinearSolver` object to use for solving the nonlinear system (2.7) or (2.5). A call to this function attaches the nonlinear solver to the main CVODE integrator.

int **CVodeSetNonlinearSolver**(void *cvode_mem, *SUNNonlinearSolver* NLS)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `NLS` – `SUNNonlinearSolver` object to use for solving nonlinear systems (2.4) or (2.5).

Return value:

- `CV_SUCCESS` – The nonlinear solver was successfully attached.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*

- `CV_ILL_INPUT` – The `SUNNonlinearSolver` object is `NULL`, does not implement the required nonlinear solver operations, is not of the correct type, or the residual function, convergence test function, or maximum number of nonlinear iterations could not be set.

5.5.7 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()*

int **CVodeRootInit**(void *cvode_mem, int nrtfn, *CVRootFn* g)

> The function CVodeRootInit specifies that the roots of a set of functions $g_i(t, y)$ are to be found while the IVP is being solved.
>
> **Arguments:**
>
> > - cvode_mem – pointer to the CVODE memory block returned by *CVodeCreate()*.
> >
> > - nrtfn – is the number of root functions g_i.
> >
> > - g – is the C function which defines the nrtfn functions $g_i(t, y)$ whose roots are sought. See *CVRootFn* for details.
>
> **Return value:**
>
> > - CV_SUCCESS – The call was successful.
> >
> > - CV_MEM_NULL – The cvode_mem argument was NULL.
> >
> > - CV_MEM_FAIL – A memory allocation failed.
> >
> > - CV_ILL_INPUT – The function g is NULL, but nrtfn > 0.
>
> **Notes:**
>
> > If a new IVP is to be solved with a call to CVodeReInit, where the new IVP has no rootfinding problem but the prior one did, then call CVodeRootInit with nrtfn=0.

5.5.8 Projection initialization function

When solving an IVP with a constraint equation, CVODE has the capability to project the solution onto the constraint manifold after each time step. To activate the projection capability with a user-defined projection function, call the following set function:

int **CVodeSetProjFn**(void *cvode_mem, *CVProjFn* proj)

> The function CVodeSetProjFn enables or disables projection with a user-defined projection function.
>
> **Arguments:**
>
> > - cvode_mem – is a pointer to the CVODE memory block returned by *CVodeCreate()*.
> >
> > - proj – is the C function which defines the projection. See *CVProjFn* for details.
>
> **Return value:**
>
> > - CV_SUCCESS – The call was successful.
> >
> > - CV_MEM_NULL – The cvode_mem argument was NULL.
> >
> > - CV_MEM_FAIL – A memory allocation failed.
> >
> > - CV_ILL_INPUT – The projection function is NULL or the method type is not CV_BDF.
>
> **Notes:**
>
> > At this time projection is only supported with BDF methods. If a new IVP is to be solved with a call to CVodeReInit, where the new IVP does not have a constraint equation but the prior one did, then call CVodeSetProjFrequency with an input of 0 to disable projection.

New in version 5.3.0.

5.5.9 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.

int **CVode**(void *cvode_mem, *realtype* tout, *N_Vector* yout, *realtype* *tret, int itask)

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

    Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `tout` – the next time at which a computed solution is desired.

- `yout` – the computed solution vector.

- `tret` – the time reached by the solver (output).

- `itask` – a flag indicating the job of the solver for the next user step. The `CV_NORMAL` option causes the solver to take internal steps until it has reached or just passed the user-specified `tout` parameter. The solver then interpolates in order to return an approximate value of $y(tout)$. The `CV_ONE_STEP` option tells the solver to take just one internal step and then return the solution at the point reached by that step.

    Return value:

- `CV_SUCCESS` – `CVode` succeeded and no roots were found.

- `CV_TSTOP_RETURN` – `CVode` succeeded by reaching the stopping point specified through the optional input function *CVodeSetStopTime()*.

- `CV_ROOT_RETURN` – `CVode` succeeded and found one or more roots. In this case, `tret` is the location of the root. If $nrtfn > 1$, call *CVodeGetRootInfo()* to see which g_i were found to have a root.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- `CV_NO_MALLOC` – The CVODE memory was not allocated by a call to *CVodeInit()*.

- `CV_ILL_INPUT` – One of the inputs to `CVode` was illegal, or some other input to the solver was illegal or missing. The latter category includes the following situations:

    (a) The tolerances have not been set.

    (b) A component of the error weight vector became zero during internal time-stepping.

    (c) The linear solver initialization function (called by the user after calling *CVodeCreate()*) failed to set the linear solver-specific `lsolve` field in `cvode_mem`.

    (d) A root of one of the root functions was found both at a point t and also very near t.

- `CV_TOO_CLOSE` – The initial time t_0 and the output time t_{out} are too close to each other and the user did not specify an initial step size.

- `CV_TOO_MUCH_WORK` – The solver took `mxstep` internal steps but still could not reach `tout`. The default value for `mxstep` is `MXSTEP_DEFAULT = 500`.

- `CV_TOO_MUCH_ACC` – The solver could not satisfy the accuracy demanded by the user for some internal step.

- `CV_ERR_FAILURE` – Either error test failures occurred too many times (`MXNEF = 7`) during one internal time step, or with $|h| = h_{min}$.

- `CV_CONV_FAILURE` – Either convergence test failures occurred too many times (`MXNCF = 10`) during one internal time step, or with $|h| = h_{min}$.

- `CV_LINIT_FAIL` – The linear solver interface's initialization function failed.

- `CV_LSETUP_FAIL` – The linear solver interface's setup function failed in an unrecoverable manner.

- `CV_LSOLVE_FAIL` – The linear solver interface's solve function failed in an unrecoverable manner.

- `CV_CONSTR_FAIL` – The inequality constraints were violated and the solver was unable to recover.

- `CV_RHSFUNC_FAIL` – The right-hand side function failed in an unrecoverable manner.

- `CV_FIRST_RHSFUNC_FAIL` – The right-hand side function had a recoverable error at the first call.

- `CV_REPTD_RHSFUNC_ERR` – Convergence test failures occurred too many times due to repeated recoverable errors in the right-hand side function. This flag will also be returned if the right-hand side function had repeated recoverable errors during the estimation of an initial step size.

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

- `CV_RTFUNC_FAIL` – The rootfinding function failed.

Notes:

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

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

If a stop time is enabled (through a call to `CVodeSetStopTime`), then `CVode` returns the solution at `tstop`. Once the integrator returns at a stop time, any future testing for `tstop` is disabled (and can be reenabled only though a new call to `CVodeSetStopTime`).

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

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

5.5.10 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. The main inputs are divided into the following categories:

- Table 5.1 lists the main CVODE optional input functions,

- Table 5.2 lists the CVLS linear solver interface optional input functions,

- Table 5.3 lists the CVNLS nonlinear solver interface optional input functions,

- Table 5.4 lists the CVODE step size adaptivity optional input functions,

- Table 5.5 lists the rootfinding optional input functions, and

- Table 5.6 lists the projection optional input functions.

These optional inputs are described in detail in the remainder of this section. Note that the diagonal linear solver module has no optional inputs. For the most casual use of CVODE, the reader can skip to §5.6.

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

The optional input calls can, unless otherwise noted, be executed in any order. However, if the user's program calls either *CVodeSetErrFile()* or *CVodeSetErrHandlerFn()*, then that call should appear first, in order to take effect for any later error message. Finally, a call to an `CVodeSet***` function can, unless otherwise noted, be made at any time from the user's calling program and, if successful, takes effect immediately.

5.5.10.1 Main solver optional input functions

Table 5.1: Optional inputs for CVODE

Optional input	Function name	Default
Pointer to an error file	*CVodeSetErrFile()*	`stderr`
Error handler function	*CVodeSetErrHandlerFn()*	internal fn.
User data	*CVodeSetUserData()*	`NULL`
Maximum order for BDF method	*CVodeSetMaxOrd()*	5
Maximum order for Adams method	*CVodeSetMaxOrd()*	12
Maximum no. of internal steps before t_{out}	*CVodeSetMaxNumSteps()*	500
Maximum no. of warnings for $t_n + h = t_n$	*CVodeSetMaxHnilWarns()*	10
Flag to activate stability limit detection	*CVodeSetStabLimDet()*	`SUNFALSE`
Initial step size	*CVodeSetInitStep()*	estimated
Minimum absolute step size	*CVodeSetMinStep()*	0.0
Maximum absolute step size	*CVodeSetMaxStep()*	∞
Value of t_{stop}	*CVodeSetStopTime()*	undefined
Interpolate at t_{stop}	*CVodeSetInterpolateStopTime()*	`SUNFALSE`
Disable the stop time	*CVodeClearStopTime()*	N/A
Maximum no. of error test failures	*CVodeSetMaxErrTestFails()*	7
Inequality constraints on solution	*CVodeSetConstraints()*	
Flag to activate specialized fused kernels	*CVodeSetUseIntegratorFusedKernels()*	`SUNFALSE`

int **CVodeSetErrFile**(void *cvode_mem, FILE *errfp)

> The function `CVodeSetErrFile` specifies a pointer to the file where all CVODE messages should be directed when the default CVODE error handler function is used.
>
> **Arguments:**
>
> - `cvode_mem` – pointer to the CVODE memory block.
>
> - `errfp` – pointer to output file.
>
> **Return value:**
>
> - `CV_SUCCESS` – The optional value has been successfully set.
>
> - `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> **Notes:**
>
> The default value for `errfp` is `stderr`. Passing a value of `NULL` disables all future error message output (except for the case in which the CVODE memory pointer is `NULL`). This use of `CVodeSetErrFile` is strongly discouraged.

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

int **CVodeSetErrHandlerFn**(void *cvode_mem, *CVErrHandlerFn* ehfun, void *eh_data)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- ehfun – is the C error handler function of type *CVErrHandlerFn*.

- eh_data – pointer to user data passed to ehfun every time it is called.

Return value:

- CV_SUCCESS – The function ehfun and data pointer eh_data have been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

int **CVodeSetUserData**(void *cvode_mem, void *user_data)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- user_data – pointer to the user data.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

> **Warning:** If user_data is needed in user linear solver or preconditioner functions, the call to CVodeSetUserData must be made before the call to specify the linear solver.

int **CVodeSetMonitorFn**(void *cvode_mem, *CVMonitorFn* monitorfn)

The function CVodeSetMonitorFn specifies a user function, monitorfn, to be called at some interval of successfully completed CVODE time steps.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- monitorfn – user-supplied monitor function (NULL by default); a NULL input will turn off monitoring

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

The frequency with which the monitor function is called can be set with the function CVodeSetMonitorFrequency.

> **Warning:** Modifying the solution in this function will result in undefined behavior. This function is only intended to be used for monitoring the integrator. SUNDIALS must be built with the CMake option SUNDIALS_BUILD_WITH_MONITORING, to utilize this function. See §11 for more information.

int **CVodeSetMonitorFrequency**(void *cvode_mem, long int nst)

The function CVodeSetMonitorFrequency specifies the interval, measured in successfully completed CVODE time-steps, at which the monitor function should be called.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nst – number of successful steps inbetween calls to the monitor function 0 by default; a 0 input will turn off monitoring.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized *CVodeCreate()*.

Notes:

The monitor function that will be called can be set with CVodeSetMonitorFn.

> **Warning:** Modifying the solution in this function will result in undefined behavior. This function is only intended to be used for monitoring the integrator. SUNDIALS must be built with the CMake option SUNDIALS_BUILD_WITH_MONITORING, to utilize this function. See §11 for more information.

int **CVodeSetMaxOrd**(void *cvode_mem, int maxord)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- maxord – value of the maximum method order. This must be positive.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_ILL_INPUT – The specified value maxord is ≤ 0, or larger than its previous value.

Notes:

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

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

int **CVodeSetMaxNumSteps**(void *cvode_mem, long int mxsteps)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `mxsteps` – maximum allowed number of steps.

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

Passing `mxsteps` = 0 results in CVODE using the default value (500).

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

int **CVodeSetMaxHnilWarns**(void *cvode_mem, int mxhnil)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `mxhnil` – maximum number of warning messages (> 0).

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

int **CVodeSetStabLimDet**(void *cvode_mem, *booleantype* stldet)

The function `CVodeSetStabLimDet` indicates if the BDF stability limit detection algorithm should be used. See §2.4 for further details.

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `stldet` – flag controlling stability limit detection (SUNTRUE = on; SUNFALSE = off)

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

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

Notes:

The default value is `SUNFALSE`. If `stldet = SUNTRUE` when BDF is used and the method order is greater

than or equal to 3, then an internal function, `CVsldet`, is called to detect a possible stability limit. If such a limit is detected, then the order is reduced.

int **CVodeSetInitStep**(void *cvode_mem, *realtype* hin)

The function `CVodeSetInitStep` specifies the initial step size.

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `hin` – value of the initial step size to be attempted. Pass 0.0 to use the default value.

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

int **CVodeSetMinStep**(void *cvode_mem, *realtype* hmin)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

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

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

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

Notes:

The default value is 0.0.

int **CVodeSetMaxStep**(void *cvode_mem, *realtype* hmax)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `hmax` – maximum absolute value of the step size (≥ 0.0).

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- `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 ∞.

int **CVodeSetStopTime**(void *cvode_mem, *realtype* tstop)

> The function CVodeSetStopTime specifies the value of the independent variable t past which the solution is not to proceed.
>
> **Arguments:**
>
> > - cvode_mem – pointer to the CVODE memory block.
> >
> > - tstop – value of the independent variable past which the solution should not proceed.
>
> **Return value:**
>
> > - CV_SUCCESS – The optional value has been successfully set.
> >
> > - CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
> >
> > - CV_ILL_INPUT – The value of tstop is not beyond the current t value, t_n.
>
> **Notes:**
>
> > The default, if this routine is not called, is that no stop time is imposed.
> >
> > Once the integrator returns at a stop time, any future testing for tstop is disabled (and can be reenabled only though a new call to CVodeSetStopTime).
> >
> > A stop time not reached before a call to *CVodeReInit()* will remain active but can be disabled by calling *CVodeClearStopTime()*.

int **CVodeSetInterpolateStopTime**(void *cvode_mem, *booleantype* interp)

> The function CVodeSetInterpolateStopTime specifies that the output solution should be interpolated when the current t equals the specified tstop (instead of merely copying the internal solution y_n).
>
> **Arguments:**
>
> > - cvode_mem – pointer to the CVODES memory block.
> >
> > - interp – flag indicating to use interpolation (1) or copy (0).
>
> **Return value:**
>
> > - CV_SUCCESS – The optional value has been successfully set.
> >
> > - CV_MEM_NULL – The CVODES memory block was not initialized through a previous call to *CVodeCreate()*.
>
> New in version 6.6.0.

int **CVodeClearStopTime**(void *cvode_mem)

> Disables the stop time set with *CVodeSetStopTime()*.
>
> **Arguments:**
>
> > - cvode_mem – pointer to the CVODE memory block.
>
> **Return value:**
>
> > - CV_SUCCESS if successful
> >
> > - CV_MEM_NULL if the CVODE memory is NULL
>
> **Notes:**
>
> > The stop time can be reenabled though a new call to *CVodeSetStopTime()*.
>
> New in version 6.5.1.

int **CVodeSetMaxErrTestFails**(void *cvode_mem, int maxnef)

> The function CVodeSetMaxErrTestFails specifies the maximum number of error test failures permitted in attempting one step.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - maxnef – maximum number of error test failures allowed on one step (> 0).
>
> **Return value:**
>
> - CV_SUCCESS – The optional value has been successfully set.
>
> - CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> **Notes:**
>
> > The default value is 7.

int **CVodeSetConstraints**(void *cvode_mem, *N_Vector* constraints)

> The function CVodeSetConstraints specifies a vector defining inequality constraints for each component of the solution vector y.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - constraints – vector of constraint flags. If constraints[i] is
>
>   - 0.0 then no constraint is imposed on y_i.
>
>   - 1.0 then y_i will be constrained to be $y_i \geq 0.0$.
>
>   - -1.0 then y_i will be constrained to be $y_i \leq 0.0$.
>
>   - 2.0 then y_i will be constrained to be $y_i > 0.0$.
>
>   - -2.0 then y_i will be constrained to be $y_i < 0.0$.
>
> **Return value:**
>
> - CV_SUCCESS – The optional value has been successfully set.
>
> - CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*
>
> - CV_ILL_INPUT – The constraints vector contains illegal values.
>
> **Notes:**
>
> > The presence of a non-NULL constraints vector that is not 0.0 in all components will cause constraint checking to be performed. However, a call with 0.0 in all components of constraints will result in an illegal input return. A NULL constraints vector will disable constraint checking.

int **CVodeSetUseIntegratorFusedKernels**(void *cvode_mem, *booleantype* onoff)

> The function CVodeSetUseIntegratorFusedKernels informs CVODE that it should use specialized fused kernels internally, if available. The specialized kernels may offer performance improvements for small problem sizes. Users should beware that these kernels can cause changes in the behavior of the integrator. By default, these kernels are not used. Must be called after *CVodeInit()*.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - onoff – boolean flag to turn on the specialized kernels (SUNTRUE), or to turn them off (SUNFALSE).

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.
- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

SUNDIALS must be compiled appropriately for specialized kernels to be available. The CMake option `SUNDIALS_BUILD_PACKAGE_FUSED_KERNELS` must be set to `ON` when SUNDIALS is compiled. See the entry for this option in §11.1.2 for more information. Currently, the fused kernels are only supported when using CVODE with the *NVECTOR_CUDA* and *NVECTOR_HIP* implementations of the `N_Vector`.

5.5.10.2 Linear solver interface optional input functions

Table 5.2: Optional inputs for the CVLS linear solver interface

Optional input	Function name	Default
Max allowed γ change without a linear solver setup	*CVodeSetDeltaGammaMaxLSetup()*	0.3
Max allowed γ change to update the Jacobian / preconditioner after a NLS failure	*CVodeSetDeltaGammaMaxBadJac()*	0.2
Linear solver setup frequency	*CVodeSetLSetupFrequency()*	20
Jacobian / preconditioner update frequency	*CVodeSetJacEvalFrequency()*	51
Jacobian function	*CVodeSetJacFn()*	DQ
Linear System function	*CVodeSetLinSysFn()*	internal
Enable or disable linear solution scaling	*CVodeSetLinearSolutionScaling()*	on
Jacobian-times-vector functions	*CVodeSetJacTimes()*	NULL, DQ
Jacobian-times-vector DQ RHS function	*CVodeSetJacTimesRhsFn()*	NULL
Preconditioner functions	*CVodeSetPreconditioner()*	NULL, NULL
Ratio between linear and nonlinear tolerances	*CVodeSetEpsLin()*	0.05
Newton linear solve tolerance conversion factor	*CVodeSetLSNormFactor()*	vector length

The mathematical explanation of the linear solver methods available to CVODE is provided in §2.1. We group the user-callable routines into four categories: general routines concerning the overall CVLS linear solver interface, optional inputs for matrix-based linear solvers, optional inputs for matrix-free linear solvers, and optional inputs for iterative linear solvers. We note that the matrix-based and matrix-free groups are mutually exclusive, whereas the "iterative" tag can apply to either case.

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

The matrix or preconditioner for M can only be updated within a call to the linear solver 'setup' routine. In general, the frequency with which this setup routine is called may be controlled with the `msbp` argument to *CVodeSetLSetupFrequency()*. When this occurs, the validity of M for successive time steps intimately depends on whether the corresponding γ and J inputs remain valid.

At each call to the linear solver setup routine the decision to update M with a new value of γ, and to reuse or reevaluate Jacobian information, depends on several factors including:

- the success or failure of previous solve attempts,

- the success or failure of the previous time step attempts,

- the change in γ from the value used when constructing M, and

- the number of steps since Jacobian information was last evaluated.

Jacobian information is considered out-of-date when $msbj$ or more steps have been completed since the last update, in which case it will be recomputed during the next linear solver setup call. The value of $msbj$ is controlled with the `msbj` argument to *CVodeSetJacEvalFrequency()*.

For linear-solvers with user-supplied preconditioning the above factors are used to determine whether to recommend updating the Jacobian information in the preconditioner (i.e., whether to set `jok` to `SUNFALSE` in calling the *user-supplied preconditioner setup function*. For matrix-based linear solvers these factors determine whether the matrix $J(t, y) = \dfrac{\partial f(t, y)}{\partial y}$ should be updated (either with an internal finite difference approximation or a call to the *user-supplied Jacobian function*; if not then the previous value is reused and the system matrix $M(t, y) \approx I - \gamma J(t, y)$ is recomputed using the current γ value.

int **CVodeSetDeltaGammaMaxLSetup**(void *cvode_mem, *realtype* dgmax_lsetup)

The function `CVodeSetDeltaGammaMaxLSetup` specifies the maximum allowed γ change that does not require a linear solver setup call. If `|gamma_current / gamma_previous - 1| > dgmax_lsetup`, the linear solver setup function is called.

If `dgmax_lsetup` is < 0, the default value (0.3) will be used.

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `dgmax_lsetup` – the γ change threshold.

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

New in version 6.2.0.

int **CVodeSetDeltaGammaMaxBadJac**(void *cvode_mem, *realtype* dgmax_jbad)

The function `CVodeSetDeltaGammaMaxBadJac` specifies the maximum allowed γ change after a NLS failure that requires updating the Jacobian / preconditioner. If `gamma_current < dgmax_jbad`, the Jacobian evaluation and/or preconditioner setup functions will be called.

Positive values of `dgmax_jbad` specify the threshold, all other values will result in using the default value (0.2).

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `dgmax_jbad` – the γ change threshold.

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

New in version 6.2.0.

int **CVodeSetLSetupFrequency**(void *cvode_mem, long int msbp)

    The function CVodeSetLSetupFrequency specifies the frequency of calls to the linear solver setup function.

    Arguments:

- cvode_mem – pointer to the CVODE memory block.

- msbp – the linear solver setup frequency.

    Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_ILL_INPUT – The frequency msbp is negative.

    Notes:

        Positive values of msbp specify the linear solver setup frequency. For example, an input of 1 means the setup function will be called every time step while an input of 2 means it will be called called every other time step. If msbp = 0, the default value of 20 will be used. Otherwise an error is returned.

int **CVodeSetJacEvalFrequency**(void *cvode_mem, long int msbj)

    The function CVodeSetJacEvalFrequency Specifies the number of steps after which the Jacobian information is considered out-of-date, $msbj$ from §2.1.1.

    Arguments:

- cvode_mem – pointer to the CVODE memory block.

- msbj – the Jacobian re-computation or preconditioner update frequency.

    Return value:

- CVLS_SUCCESS – The optional value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver interface has not been initialized.

- CVLS_ILL_INPUT – The frequency msbj is negative.

    Notes:

        If nstlj is the step number at which the Jacobian information was lasted updated and nst is the current step number, nst - nstlj >= msbj indicates the Jacobian information will be updated during the next linear solver setup call.

        As the Jacobian update frequency is only checked *within* calls to the linear solver setup routine, Jacobian information may be more than msbj steps old when updated depending on when a linear solver setup call occurs. See §2.1.1 for more information on when linear solver setups are performed.

        If msbj = 0, the default value of 51 will be used. Otherwise an error is returned.

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

When using matrix-based linear solver modules, the CVLS solver interface needs a function to compute an approximation to the Jacobian matrix $J(t, y)$ or the linear system $M = I - \gamma J$. The function to evaluate $J(t, y)$ must be of type *CVLsJacFn*. The user can supply a Jacobian function, or if using a *SUNMATRIX_DENSE* or *SUNMATRIX_BAND* matrix J, can use the default internal difference quotient approximation that comes with the CVLS solver. To specify a user-supplied Jacobian function jac, CVLS provides the function *CVodeSetJacFn()*. The CVLS interface passes the pointer user_data to the Jacobian function. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied Jacobian function, without using global data in the program. The pointer user_data may be specified through *CVodeSetUserData()*.

int **CVodeSetJacFn**(void *cvode_mem, *CVLsJacFn* jac)

> The function CVodeSetJacFn specifies the Jacobian approximation function to be used for a matrix-based solver within the CVLS interface.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - jac – user-defined Jacobian approximation function.
>
> **Return value:**
>
> - CVLS_SUCCESS – The optional value has been successfully set.
>
> - CVLS_MEM_NULL – The cvode_mem pointer is NULL.
>
> - CVLS_LMEM_NULL – The CVLS linear solver interface has not been initialized.
>
> **Notes:**
>
> > This function must be called after the CVLS linear solver interface has been initialized through a call to *CVodeSetLinearSolver()*.
> >
> > By default, CVLS uses an internal difference quotient function for the *SUNMATRIX_DENSE* and *SUN-MATRIX_BAND* modules. If NULL is passed to jac, this default function is used. An error will occur if no jac is supplied when using other matrix types.
> >
> > The function type *CVLsJacFn* is described in §5.6.7.
> >
> > The previous routine CVDlsSetJacFn is now a wrapper for this routine, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

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

int **CVodeSetLinSysFn**(void *cvode_mem, *CVLsLinSysFn* linsys)

> The function CVodeSetLinSysFn specifies the linear system approximation function to be used for a matrix-based solver within the CVLS interface.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - linsys – user-defined linear system approximation function.
>
> **Return value:**
>
> - CVLS_SUCCESS – The optional value has been successfully set.
>
> - CVLS_MEM_NULL – The cvode_mem pointer is NULL.
>
> - CVLS_LMEM_NULL – The CVLS linear solver interface has not been initialized.
>
> **Notes:**
>
> > This function must be called after the CVLS linear solver interface has been initialized through a call to *CVodeSetLinearSolver()*.
> >
> > By default, CVLS uses an internal linear system function leveraging the SUNMatrix API to form the system $M = I - \gamma J$ using either an internal finite difference approximation or user-supplied function to compute the Jacobian. If linsys is NULL, this default function is used.
> >
> > The function type *CVLsLinSysFn* is described in §5.6.7.

When using a matrix-based linear solver the matrix information will be updated infrequently to reduce matrix construction and, with direct solvers, factorization costs. As a result the value of γ may not be current and, with BDF methods, a scaling factor is applied to the solution of the linear system to account for the lagged value of γ. See §8.2.1 for more details. The function *CVodeSetLinearSolutionScaling()* can be used to disable this scaling when necessary, e.g., when providing a custom linear solver that updates the matrix using the current γ as part of the solve.

int **CVodeSetLinearSolutionScaling**(void *cvode_mem, *booleantype* onoff)

> The function *CVodeSetLinearSolutionScaling()* enables or disables scaling the linear system solution to account for a change in γ in the linear system. For more details see §8.2.1.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - onoff – flag to enable (SUNTRUE) or disable (SUNFALSE) scaling.
>
> **Return value:**
>
> - CVLS_SUCCESS – The flag value has been successfully set.
>
> - CVLS_MEM_NULL – The cvode_mem pointer is NULL.
>
> - CVLS_LMEM_NULL – The CVLS linear solver interface has not been initialized.
>
> - CVLS_ILL_INPUT – The attached linear solver is not matrix-based or the linear multistep method type is not BDF.
>
> **Notes:**
>
> > This function must be called after the CVLS linear solver interface has been initialized through a call to CVodeSetLinearSolver.
> >
> > By default scaling is enabled with matrix-based linear solvers when using BDF methods.

When using matrix-free linear solver modules, the CVLS solver interface requires a function to compute an approximation to the product between the Jacobian matrix $J(t, y)$ and a vector v. The user can supply a Jacobian-times-vector approximation function or use the default internal difference quotient function that comes with the CVLS interface.

A user-defined Jacobian-vector product function must be of type *CVLsJacTimesVecFn* and can be specified through a call to *CVodeSetJacTimes()* (see §5.6.9 for specification details). The evaluation and processing of any Jacobian-related data needed by the user's Jacobian-times-vector function may be done in the optional user-supplied function jtsetup (see §5.6.10 for specification details). The pointer user_data received through *CVodeSetUserData()* (or a pointer to NULL if user_data was not specified) is passed to the Jacobian-times-vector setup and product functions, jtsetup and jtimes, each time they are called. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied functions without using global data in the program.

int **CVodeSetJacTimes**(void *cvode_mem, *CVLsJacTimesSetupFn* jtsetup, *CVLsJacTimesVecFn* jtimes)

> The function CVodeSetJacTimes specifies the Jacobian-vector setup and product functions.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
>
> - jtsetup – user-defined Jacobian-vector setup function of type *CVLsJacTimesSetupFn*.
>
> - jtimes – user-defined Jacobian-vector product function of type *CVLsJacTimesVecFn*.
>
> **Return value:**
>
> - CVLS_SUCCESS – The optional value has been successfully set.
>
> - CVLS_MEM_NULL – The cvode_mem pointer is NULL.
>
> - CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

- CVLS_SUNLS_FAIL – An error occurred when setting up the system matrix-times-vector routines in the SUNLinearSolver object used by the CVLS interface.

Notes:

The default is to use an internal finite difference quotient for jtimes and to omit jtsetup. If NULL is passed to jtimes, these defaults are used. A user may specify non-NULL jtimes and NULL jtsetup inputs.

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

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

When using the internal difference quotient the user may optionally supply an alternative right-hand side function for use in the Jacobian-vector product approximation by calling *CVodeSetJacTimesRhsFn()*. The alternative right-hand side function should compute a suitable (and differentiable) approximation to the right-hand side function provided to *CVodeInit()*. For example, as done in [27], the alternative function may use lagged values when evaluating a nonlinearity in the right-hand side to avoid differencing a potentially non-differentiable factor.

int **CVodeSetJacTimesRhsFn**(void *cvode_mem, *CVRhsFn* jtimesRhsFn)

The function CVodeSetJacTimesRhsFn specifies an alternative ODE right-hand side function for use in the internal Jacobian-vector product difference quotient approximation.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- jtimesRhsFn – is the C function which computes the alternative ODE right-hand side function to use in Jacobian-vector product difference quotient approximations. This function has the form f(t, y, ydot, user_data) (for full details see *CVRhsFn*).

Return value:

- CVLS_SUCCESS – The optional value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

- CVLS_ILL_INPUT – The internal difference quotient approximation is disabled.

Notes:

The default is to use the right-hand side function provided to *CVodeInit()* in the internal difference quotient. If the input right-hand side function is NULL, the default is used.

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

When using an iterative linear solver, the user may supply a preconditioning operator to aid in solution of the system. This operator consists of two user-supplied functions, psetup and psolve, that are supplied to CVODE using the function *CVodeSetPreconditioner()*. The psetup function supplied to this routine should handle evaluation and preprocessing of any Jacobian data needed by the user's preconditioner solve function, psolve. The user data pointer received through *CVodeSetUserData()* (or a pointer to NULL if user data was not specified) is passed to the psetup and psolve functions. This allows the user to create an arbitrary structure with relevant problem data and access it during the execution of the user-supplied preconditioner functions without using global data in the program.

Also, as described in §2.1, the CVLS interface requires that iterative linear solvers stop when the norm of the preconditioned residual satisfies

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

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

int **CVodeSetPreconditioner**(void *cvode_mem, *CVLsPrecSetupFn* psetup, *CVLsPrecSolveFn* psolve)

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

>   **Arguments:**

>>   - cvode_mem – pointer to the CVODE memory block.

>>   - psetup – user-defined preconditioner setup function. Pass NULL if no setup is necessary.

>>   - psolve – user-defined preconditioner solve function.

>   **Return value:**

>>   - CVLS_SUCCESS – The optional values have been successfully set.

>>   - CVLS_MEM_NULL – The cvode_mem pointer is NULL.

>>   - CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

>>   - CVLS_SUNLS_FAIL – An error occurred when setting up preconditioning in the SUNLinearSolver object used by the CVLS interface.

>   **Notes:**

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

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

>>   The function type *CVLsPrecSolveFn* is described in §5.6.11.

>>   The function type *CVLsPrecSetupFn* is described in §5.6.12

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

int **CVodeSetEpsLin**(void *cvode_mem, *realtype* eplifac)

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

>   **Arguments:**

>>   - cvode_mem – pointer to the CVODE memory block.

>>   - eplifac – linear convergence safety factor (≥ 0).

>   **Return value:**

>>   - CVLS_SUCCESS – The optional value has been successfully set.

>>   - CVLS_MEM_NULL – The cvode_mem pointer is NULL.

>>   - CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

>>   - CVLS_ILL_INPUT – The factor eplifac is negative.

>   **Notes:**

>>   The default value is 0.05.

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

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

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

int **CVodeSetLSNormFactor**(void *cvode_mem, *realtype* nrmfac)

The function `CVodeSetLSNormFactor` specifies the factor to use when converting from the integrator tolerance (WRMS norm) to the linear solver tolerance (L2 norm) for Newton linear system solves e.g., `tol_L2 = fac * tol_WRMS`.

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `nrmfac` – the norm conversion factor. If `nrmfac` is:

    - > 0 then the provided value is used.

    - $= 0$ then the conversion factor is computed using the vector length, i.e., `nrmfac = N_-VGetLength(y)` (*default*).

    - < 0 then the conversion factor is computed using the vector dot product, i.e., `nrmfac = N_-VDotProd(v,v)` where all the entries of `v` are one.

Return value:

- `CV_SUCCESS` – The optional value has been successfully set.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

Prior to the introduction of `N_VGetLength` in SUNDIALS v5.0.0 (CVODE v5.0.0) the value of `nrmfac` was computed using the vector dot product i.e., the `nrmfac < 0` case.

5.5.10.3 Nonlinear solver interface optional input functions

Table 5.3: Optional inputs for the CVNLS nonlinear solver interface

Optional input	Function name	Default
Maximum no. of nonlinear iterations	*CVodeSetMaxNonlinIters()*	3
Maximum no. of convergence failures	*CVodeSetMaxConvFails()*	10
Coefficient in the nonlinear convergence test	*CVodeSetNonlinConvCoef()*	0.1
ODE RHS function for nonlinear system evaluations	*CVodeSetNlsRhsFn()*	NULL

The following functions can be called to set optional inputs controlling the nonlinear solver.

int **CVodeSetMaxNonlinIters**(void *cvode_mem, int maxcor)

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

Arguments:

- `cvode_mem` – pointer to the CVODE memory block.

- `maxcor` – maximum number of nonlinear solver iterations allowed per step (> 0).

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_MEM_FAIL – The SUNNonlinearSolver module is NULL.

Notes:
The default value is 3.

int **CVodeSetMaxConvFails**(void *cvode_mem, int maxncf)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- maxncf – maximum number of allowable nonlinear solver convergence failures per step (> 0).

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:
The default value is 10.

int **CVodeSetNonlinConvCoef**(void *cvode_mem, *realtype* nlscoef)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nlscoef – coefficient in nonlinear convergence test (> 0).

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:
The default value is 0.1.

int **CVodeSetNlsRhsFn**(void *cvode_mem, *CVRhsFn* f)

The function CVodeSetNlsRhsFn specifies an alternative right-hand side function for use in nonlinear system function evaluations.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- f – is the alternative C function which computes the right-hand side function f in the ODE (for full details see *CVRhsFn*).

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

The default is to use the implicit right-hand side function provided to *CVodeInit()* in nonlinear system function evaluations. If the input right-hand side function is NULL, the default is used.

When using a non-default nonlinear solver, this function must be called after *CVodeSetNonlinearSolver()*.

5.5.10.4 Time step adaptivity optional input functions

Table 5.4: Optional inputs for CVODE time step adaptivity

Optional input	Function name	Default
Fixed step size factor bounds $\eta_{\text{min\_fx}}$ and $\eta_{\text{max\_fx}}$	*CVodeSetEtaFixedStepBounds()*	0 and 1.5
Largest allowed step size change factor in the first step $\eta_{\text{max\_fs}}$	*CVodeSetEtaMaxFirstStep()*	10^4
Largest allowed step size change factor for early steps $\eta_{\text{max\_es}}$	*CVodeSetEtaMaxEarlyStep()*	10
Number of time steps to use the early step size change factor	*CVodeSetNumStepsEtaMaxEarlyStep()*	10
Largest allowed step size change factor after a successful step $\eta_{\text{max\_gs}}$	*CVodeSetEtaMax()*	10
Smallest allowed step size change factor after a successful step η_{min}	*CVodeSetEtaMin()*	1.0
Smallest allowed step size change factor after an error test fail $\eta_{\text{min\_ef}}$	*CVodeSetEtaMinErrFail()*	0.1
Largest allowed step size change factor after multiple error test fails $\eta_{\text{max\_ef}}$	*CVodeSetEtaMaxErrFail()*	0.2
Number of error failures necessary for $\eta_{\text{max\_ef}}$	*CVodeSetNumFailsEtaMaxErrFail()*	2
Step size change factor after a nonlinear solver convergence failure η_{cf}	*CVodeSetEtaConvFail()*	0.25

The following functions can be called to set optional inputs to control the step size adaptivity.

Note: The default values for the step size adaptivity tuning parameters have a long history of success and changing the values is generally discouraged. However, users that wish to experiment with alternative values should be careful to make changes gradually and with testing to determine their effectiveness.

---

int **CVodeSetEtaFixedStepBounds**(void *cvode_mem, *realtype* eta_min_fx, *realtype* eta_max_fx)

The function CVodeSetEtaFixedStepBounds specifies the interval lower ($\eta_{\text{min\_fx}}$) and upper ($\eta_{\text{max\_fx}}$) bounds in which the step size will remain unchanged i.e., if $\eta_{\text{min\_fx}} < \eta < \eta_{\text{max\_fx}}$, then $\eta = 1$.

The default values are $\eta_{\text{min\_fx}} = 0$ and $\eta_{\text{max\_fx}} = 1.5$

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_min_fx – value of the lower bound of the fixed step interval. If eta_min_fx is < 0 or ≥ 1, the default value is used.

- eta_max_fx – value of the upper bound of the fixed step interval. If eta_max_fx is < 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

New in version 6.2.0.

int **CVodeSetEtaMaxFirstStep**(void *cvode_mem, *realtype* eta_max_fs)

The function CVodeSetEtaMaxFirstStep specifies the maximum step size factor after the first time step, $\eta_{\text{max\_fs}}$.

The default value is $\eta_{\text{max\_fs}} = 10^4$.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_max_fs – value of the maximum step size factor after the first time step. If eta_max_fs is ≤ 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

New in version 6.2.0.

int **CVodeSetEtaMaxEarlyStep**(void *cvode_mem, *realtype* eta_max_es)

The function CVodeSetEtaMaxEarlyStepEtaMax specifies the maximum step size factor for steps early in the integration, $\eta_{\text{max\_es}}$.

The default value is $\eta_{\text{max\_es}} = 10$.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_max_es – value of the maximum step size factor for early in the integration. If eta_max_es is ≤ 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Note: The factor for the first time step is set by *CVodeSetEtaMaxFirstStep()*.

The number of time steps that use the early integration maximum step size factor $\eta_{\text{max\_es}}$ can be set with *CVodeSetNumStepsEtaMaxEarlyStep()*.

New in version 6.2.0.

int **CVodeSetNumStepsEtaMaxEarlyStep**(void *cvode_mem, long int small_nst)

> The function CVodeSetNumStepsEtaMaxEarlyStep specifies the number of steps to use the early integration maximum step size factor, $\eta_{\mathrm{max\_es}}$.
>
> The default value is 10.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * small_nst – value of the maximum step size factor for early in the integration. If small_nst is < 0, the default value is used. If the small_nst is 0, then the value set by *CVodeSetEtaMax()* is used.
>
> **Return value:**
>
> > * CV_SUCCESS – The optional value has been successfully set.
> >
> > * CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> ---
>
> **Note:** The factor $\eta_{\mathrm{max\_es}}$ can be set with *CVodeSetEtaMaxEarlyStep()*.
>
> ---
>
> New in version 6.2.0.

int **CVodeSetEtaMax**(void *cvode_mem, *realtype* eta_max_gs)

> The function CVodeSetEtaMax specifies the maximum step size factor, $\eta_{\mathrm{max\_gs}}$.
>
> The default value is $\eta_{\mathrm{max\_gs}} = 10$.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * eta_max_gs – value of the maximum step size factor. If eta_max_gs is ≤ 1, the default value is used.
>
> **Return value:**
>
> > * CV_SUCCESS – The optional value has been successfully set.
> >
> > * CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> ---
>
> **Note:** The factor for the first time step is set by *CVodeSetEtaMaxFirstStep()*.
>
> The factor for steps early in the integration is set by *CVodeSetEtaMaxEarlyStep()*.
>
> ---
>
> New in version 6.2.0.

int **CVodeSetEtaMin**(void *cvode_mem, *realtype* eta_min)

> The function CVodeSetEtaMin specifies the minimum step size factor, η_{min}.
>
> The default value is $\eta_{\mathrm{min}} = 1.0$.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * eta_min – value of the minimum step size factor. If eta_min is ≤ 0 or ≥ 1, the default value is used.
>
> **Return value:**
>
> > * CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

New in version 6.2.0.

int **CVodeSetEtaMinErrFail**(void *cvode_mem, *realtype* eta_min_ef)

The function CVodeSetEtaMinErrFail specifies the minimum step size factor after an error test failure, $\eta_{\min\_ef}$.

The default value is $\eta_{\min\_ef} = 0.1$.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_min_ef – value of the minimum step size factor after an error test failure. If eta_min_ef is ≤ 0 or ≥ 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

New in version 6.2.0.

int **CVodeSetEtaMaxErrFail**(void *cvode_mem, *realtype* eta_max_ef)

The function CVodeSetEtaMaxErrFail specifies the maximum step size factor after multiple error test failures, $\eta_{\max\_ef}$.

The default value is $\eta_{\min\_ef} = 0.2$.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_max_ef – value of the maximum step size factor after an multiple error test failures. If eta_-min_ef is ≤ 0 or ≥ 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

Note: The number of error test failures necessary to enforce the maximum step size factor $\eta_{\min\_ef}$ can be set with *CVodeSetNumFailsEtaMaxErrFail()*.

New in version 6.2.0.

int **CVodeSetNumFailsEtaMaxErrFail**(void *cvode_mem, int small_nef)

The function CVodeSetNumFailsEtaMaxErrFail specifies the number of error test failures necessary to enforce the maximum step size factor $\eta_{\max\_ef}$.

The default value is 2.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- small_nst – value of the maximum step size factor for early in the integration. If small_nst is < 0, the default value is used. If the small_nst is 0, then the value set by *CVodeSetEtaMax()* is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Note: The factor $\eta_{\mathrm{max\_ef}}$ can be set with *CVodeSetEtaMaxErrFail()*.

New in version 6.2.0.

int **CVodeSetEtaConvFail**(void *cvode_mem, *realtype* eta_cf)

The function CVodeSetEtaConvFail specifies the step size factor after a nonlinear solver failure η_{cf}.

The default value is $\eta_{\mathrm{cf}} = 0.25$.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eta_cf – value of the maximum step size factor after a nonlinear solver failure. If eta_cf is ≤ 0 or ≥ 1, the default value is used.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

New in version 6.2.0.

5.5.10.5 Rootfinding optional input functions

Table 5.5: Optional inputs for CVODE step size adaptivity

Optional input	**Function name**	**Default**
Direction of zero-crossing	*CVodeSetRootDirection()*	both
Disable rootfinding warnings	*CVodeSetNoInactiveRootWarn()*	none

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

int **CVodeSetRootDirection**(void *cvode_mem, int *rootdir)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- rootdir – state array of length nrtfn, the number of root functions g_i, as specified in the call to the function *CVodeRootInit()*. A value of 0 for rootdir[i] indicates that crossing in either direction for g_i should be reported. A value of $+1$ or -1 indicates that the solver should report only zero-crossings where g_i is increasing or decreasing, respectively.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_ILL_INPUT – rootfinding has not been activated through a call to *CVodeRootInit()*.

Notes:

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

int **CVodeSetNoInactiveRootWarn**(void *cvode_mem)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

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.

5.5.10.6 Projection optional input functions

Table 5.6: Optional inputs for the CVODE projection interface

Optional input	Function name	Default
Enable or disable error estimate projection	*CVodeSetProjErrEst()*	SUNTRUE
Projection frequency	*CVodeSetProjFrequency()*	1
Maximum number of projection failures	*CVodeSetMaxNumProjFails()*	10
Projection solve tolerance	*CVodeSetEpsProj()*	0.1
Step size reduction factor after a failed projection	*CVodeSetProjFailEta()*	0.25

The following functions can be called to set optional inputs to control the projection when solving an IVP with constraints.

int **CVodeSetProjErrEst**(void *cvode_mem, *booleantype* onoff)

The function CVodeSetProjErrEst enables or disables projection of the error estimate by the projection function.

Arguments:

- cvode_mem – is a pointer to the CVODE memory block.

- onoff – is a flag indicating if error projection should be enabled (SUNTRUE) or disabled (SUNFALSE).

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

int **CVodeSetProjFrequency**(void *cvode_mem, long int freq)

The function CVodeSetProjFrequency specifies the frequency with which the projection is performed.

Arguments:

- cvode_mem – is a pointer to the CVODE memory block.

- freq – is the frequency with which to perform the projection. The default is 1 (project every step), a value of 0 will disable projection, and a value < 0 will restore the default.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

int **CVodeSetMaxNumProjFails**(void *cvode_mem, int max_fails)

The function CVodeSetMaxNumProjFails specifies the maximum number of projection failures in a step attempt before an unrecoverable error is returned.

Arguments:

- cvode_mem – is a pointer to the CVODE memory block.

- max_fails – is the maximum number of projection failures. The default is 10 and an input value < 1 will restore the default.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

int **CVodeSetEpsProj**(void *cvode_mem, *realtype* eps)

The function CVodeSetEpsProj specifies the tolerance for the nonlinear constrained least squares problem solved by the projection function.

Arguments:

- cvode_mem – is a pointer to the CVODE memory block.

- eps – is the tolerance (default 0.1) for the the nonlinear constrained least squares problem solved by the projection function. A value ≤ 0 will restore the default.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

int **CVodeSetProjFailEta**(void *cvode_mem, *realtype* eta)

The function CVodeSetProjFailEta specifies the time step reduction factor to apply on a projection function failure.

Arguments:

- cvode_mem – is a pointer to the CVODE memory block.

- eps – is the time step reduction factor to apply on a projection function failure (default 0.25). A value ≤ 0 or > 1 will restore the default.

Return value:

- CV_SUCCESS – The optional value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

5.5.11 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 function has the following form:

int **CVodeGetDky**(void *cvode_mem, *realtype* t, int k, *N_Vector* dky)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- t – the value of the independent variable at which the derivative is to be evaluated.

- k – the derivative order requested.

- dky – vector containing the derivative. This vector must be allocated by the user.

Return value:

- CV_SUCCESS – CVodeGetDky succeeded.

- CV_BAD_K – k is not in the range $0, 1, \ldots, q_u$.

- CV_BAD_T – t is not in the interval $[t_n - h_u, t_n]$.

- CV_BAD_DKY – The dky argument was NULL.

- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to `CVodeCre-ate()`.

Notes:

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

5.5.12 Optional output functions

CVODE provides an extensive set of functions that can be used to obtain solver performance information. Table 5.7 lists all optional output functions in CVODE, which are then described in detail in the remainder of this section.

Some of the optional outputs, especially the various counters, can be very useful in determining how successful the CVODE solver is in doing its job. For example, the counters `nsteps` and `nfevals` provide a rough measure of the overall cost of a given run, and can be compared among runs with differing input options to suggest which set of options is most efficient. The ratio `nniters/nsteps` measures the performance of the nonlinear solver in solving the nonlinear systems at each time step; typical values for this range from 1.1 to 1.8. The ratio `njevals/nniters` (in the case of a matrix-based linear solver), and the ratio `npevals/nniters` (in the case of an iterative linear solver) measure the overall degree of nonlinearity in these systems, and also the quality of the approximate Jacobian or preconditioner being used. Thus, for example, `njevals/nniters` can indicate if a user-supplied Jacobian is inaccurate, if this ratio is larger than for the case of the corresponding internal Jacobian. The ratio `nliters/nniters` measures the performance of the Krylov iterative linear solver, and thus (indirectly) the quality of the preconditioner.

Table 5.7: Optional outputs from CVODE, CVLS, and CVDIAG

Optional output	Function name
CVODE main solver	
Size of CVODE real and integer workspaces	`CVodeGetWorkSpace()`
Cumulative number of internal steps	`CVodeGetNumSteps()`
No. of calls to r.h.s. function	`CVodeGetNumRhsEvals()`
No. of calls to linear solver setup function	`CVodeGetNumLinSolvSetups()`
No. of local error test failures that have occurred	`CVodeGetNumErrTestFails()`
No. of failed steps due to a nonlinear solver failure	`CVodeGetNumStepSolveFails()`
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()`
User data pointer	`CVodeGetUserData()`
Array showing roots found	`CVodeGetRootInfo()`
No. of calls to user root function	`CVodeGetNumGEvals()`
Print all statistics	`CVodePrintAllStats()`
Name of constant associated with a return flag	`CVodeGetReturnFlagName()`

continues on next page

Table 5.7 – continued from previous page

Optional output	Function name
CVLS linear solver interface	
Stored Jacobian of the ODE RHS function	*CVodeGetJac()*
Time at which the Jacobian was evaluated	*CVodeGetJacTime()*
Step number at which the Jacobian was evaluated	*CVodeGetJacNumSteps()*
Size of real and integer workspaces	*CVodeGetLinWorkSpace()*
No. of Jacobian evaluations	*CVodeGetNumJacEvals()*
No. of r.h.s. calls for finite diff. Jacobian[-vector] evals.	*CVodeGetNumLinRhsEvals()*
No. of linear iterations	*CVodeGetNumLinIters()*
No. of linear convergence failures	*CVodeGetNumLinConvFails()*
No. of preconditioner evaluations	*CVodeGetNumPrecEvals()*
No. of preconditioner solves	*CVodeGetNumPrecSolves()*
No. of Jacobian-vector setup evaluations	*CVodeGetNumJTSetupEvals()*
No. of Jacobian-vector product evaluations	*CVodeGetNumJtimesEvals()*
Get all linear solver statistics in one function call	*CVodeGetLinSolvStats()*
Last return from a linear solver function	*CVodeGetLastLinFlag()*
Name of constant associated with a return flag	*CVodeGetLinReturnFlagName()*
CVDIAG linear solver interface	
Size of CVDIAG real and integer workspaces	*CVDiagGetWorkSpace()*
No. of r.h.s. calls for finite diff. Jacobian evals.	*CVDiagGetNumRhsEvals()*
Last return from a CVDIAG function	*CVDiagGetLastFlag()*
Name of constant associated with a return flag	*CVDiagGetReturnFlagName()*

5.5.12.1 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.

int **CVodeGetWorkSpace**(void *cvode_mem, long int *lenrw, long int *leniw)

> The function CVodeGetWorkSpace returns the CVODE real and integer workspace sizes.
>
> **Arguments:**
>
> - cvode_mem – pointer to the CVODE memory block.
> - lenrw – the number of realtype values in the CVODE workspace.
> - leniw – the number of integer values in the CVODE workspace.
>
> **Return value:**
>
> - CV_SUCCESS – The optional output values have been successfully set.
> - CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
>
> **Notes:**
>
> In terms of the problem size N, the maximum method order maxord, and the number nrtfn of root functions (see §5.5.7) the actual size of the real workspace, in realtype words, is given by the following:
>
> - base value: lenrw $= 96 + (\text{maxord} + 5)N_r + 3\text{nrtfn}$;

- using *CVodeSVtolerances()*: $\text{lenrw} = \text{lenrw} + N_r$;

- with constraint checking (see *CVodeSetConstraints()*): $\text{lenrw} = \text{lenrw} + N_r$;

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

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

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

- using *CVodeSVtolerances()*: $\text{leniw} = \text{leniw} + N_i$;

- with constraint checking: $\text{lenrw} = \text{lenrw} + N_i$;

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

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

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

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

int **CVodeGetNumSteps**(void *cvode_mem, long int *nsteps)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nsteps – number of steps taken by CVODE.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetNumRhsEvals**(void *cvode_mem, long int *nfevals)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nfevals – number of calls to the user's f function.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

int **CVodeGetNumLinSolvSetups**(void *cvode_mem, long int *nlinsetups)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nlinsetups – number of calls made to the linear solver setup function.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetNumErrTestFails**(void *cvode_mem, long int *netfails)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- netfails – number of error test failures.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetNumStepSolveFails**(void *cvode_mem, long int *ncnf)

Returns the number of failed steps due to a nonlinear solver failure.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- ncnf – number of step failures.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetLastOrder**(void *cvode_mem, int *qlast)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- qlast – method order used on the last internal step.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetCurrentOrder**(void *cvode_mem, int *qcur)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- qcur – method order to be used on the next internal step.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetLastStep**(void *cvode_mem, *realtype* *hlast)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- hlast – step size taken on the last internal step.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetCurrentStep**(void *cvode_mem, *realtype* *hcur)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- hcur – step size to be attempted on the next internal step.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetActualInitStep**(void *cvode_mem, *realtype* *hinused)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- hinused – actual value of initial step size.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

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.

int **CVodeGetCurrentTime**(void *cvode_mem, *realtype* *tcur)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- tcur – current internal time reached.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetNumStabLimOrderReds**(void *cvode_mem, long int *nslred)

The function CVodeGetNumStabLimOrderReds returns the number of order reductions dictated by the BDF stability limit sdetection algorithm (see §2.4).

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nslred – number of order reductions due to stability limit detection.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

Notes:

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

int **CVodeGetTolScaleFactor**(void *cvode_mem, *realtype* *tolsfac)

The function CVodeGetTolScaleFactor returns a suggested factor by which the user's tolerances should be scaled when too much accuracy has been requested for some internal step.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- tolsfac – suggested scaling factor for user-supplied tolerances.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

int **CVodeGetErrWeights**(void *cvode_mem, *N_Vector* eweight)

The function CVodeGetErrWeights returns the solution error weights at the current time. These are the reciprocals of the W_i given by (2.6).

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- eweight – solution error weights at the current time.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

> **Warning:** The user must allocate memory for `eweight`.

int **CVodeGetEstLocalErrors**(void *cvode_mem, *N_Vector* ele)

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

   Arguments:

   - `cvode_mem` – pointer to the CVODE memory block.

   - `ele` – estimated local errors.

   Return value:

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

   - `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

   > **Warning:** The user must allocate memory for `ele`.
   >
   > The values returned in `ele` are valid only if *CVode()* returned a non-negative value.
   >
   > The `ele` vector, togther with the `eweight` vector from *CVodeGetErrWeights()*, can be used to determine how the various components of the system contributed to the estimated local error test. Specifically, that error test uses the RMS norm of a vector whose components are the products of the components of these two vectors. Thus, for example, if there were recent error test failures, the components causing the failures are those with largest values for the products, denoted loosely as `eweight[i]*ele[i]`.

int **CVodeGetIntegratorStats**(void *cvode_mem, long int *nsteps, long int *nfevals, long int *nlinsetups, long int *netfails, int *qlast, int *qcur, *realtype* *hinused, *realtype* *hlast, *realtype* *hcur, *realtype* *tcur)

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

   Arguments:

   - `cvode_mem` – pointer to the CVODE memory block.

   - `nsteps` – number of steps taken by CVODE.

   - `nfevals` – number of calls to the user's `f` function.

   - `nlinsetups` – number of calls made to the linear solver setup function.

   - `netfails` – number of error test failures.

   - `qlast` – method order used on the last internal step.

   - `qcur` – method order to be used on the next internal step.

   - `hinused` – actual value of initial step size.

   - `hlast` – step size taken on the last internal step.

   - `hcur` – step size to be attempted on the next internal step.

   - `tcur` – current internal time reached.

   Return value:

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

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

int **CVodeGetNumNonlinSolvIters**(void *cvode_mem, long int *nniters)

The function CVodeGetNumNonlinSolvIters returns the number of nonlinear iterations performed.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nniters – number of nonlinear iterations performed.

Return value:

- CV_SUCCESS – The optional output values have been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

- CV_MEM_FAIL – The SUNNonlinearSolver module is NULL

int **CVodeGetNumNonlinSolvConvFails**(void *cvode_mem, long int *nncfails)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nncfails – number of nonlinear convergence failures.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

int **CVodeGetNonlinSolvStats**(void *cvode_mem, long int *nniters, long int *nncfails)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nniters – number of nonlinear iterations performed.

- nncfails – number of nonlinear convergence failures.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

- CV_MEM_FAIL – The SUNNonlinearSolver module is NULL

int **CVodeGetUserData**(void *cvode_mem, void **user_data)

The function CVodeGetUserData returns the user data pointer provided to *CVodeSetUserData()*.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- user_data – memory reference to a user data pointer.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.
- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.

New in version 6.3.0.

int **CVodePrintAllStats**(void *cvode_mem, FILE *outfile, *SUNOutputFormat* fmt)

The function CVodePrintAllStats outputs all of the integrator, nonlinear solver, linear solver, and other statistics.

Arguments:

- cvode_mem – pointer to the CVODE memory block.
- outfile – pointer to output file.
- fmt – the output format:
  - *SUN_OUTPUTFORMAT_TABLE* – prints a table of values
  - *SUN_OUTPUTFORMAT_CSV* – prints a comma-separated list of key and value pairs e.g., key1, value1,key2,value2,...

Return value:

- CV_SUCCESS – The output was successfully.
- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCre-ate()*.
- CV_ILL_INPUT – An invalid formatting option was provided.

Note: The file scripts/sundials_csv.py provides python utility functions to read and output the data from a SUNDIALS CSV output file using the key and value pair format.

New in version 6.2.0.

char ***CVodeGetReturnFlagName**(int flag)

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

Arguments:

- flag – return flag from a CVODE function.

Return value:

- A string containing the name of the corresponding constant

5.5.12.2 Rootfinding optional output functions

There are two optional output functions associated with rootfinding.

int **CVodeGetRootInfo**(void *cvode_mem, int *rootsfound)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

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

Return value:

- CV_SUCCESS – The optional output values have been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

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. A value of 0 indicates that either no root was found for g_i, or that g_i varies in the direction opposite to that indicated by rootdir[i] in the case that *CVodeSetRootDirection()* was used to only track zero-crossings in one direction.

> **Warning:** The user must allocate memory for the vector rootsfound.

int **CVodeGetNumGEvals**(void *cvode_mem, long int *ngevals)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- ngevals – number of calls made to the user's function g thus far.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

5.5.12.3 Projection optional output functions

The following optional output functions are available for retrieving information and statistics related the projection when solving an IVP with constraints.

int **CVodeGetNumProjEvals**(void *cvode_mem, long int *nproj)

The function CVodeGetNumProjEvals returns the current total number of projection evaluations.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nproj – the number of calls to the projection function.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

- CV_MEM_NULL – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

- CV_PROJ_MEM_NULL – The projection memory is NULL i.e., the projection functionality has not been enabled.

New in version 5.3.0.

int **CVodeGetNumProjFails**(void *cvode_mem, long int *npfails)

> The function `CVodeGetNumProjFails` returns the current total number of projection evaluation failures.

> **Arguments:**

> - `cvode_mem` – pointer to the CVODE memory block.

> - `npfails` – the number of projection failures.

> **Return value:**

> - `CV_SUCCESS` – The optional output value has been successfully set.

> - `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.

> - `CV_PROJ_MEM_NULL` – The projection memory is NULL, i.e., the projection functionality has not been enabled.

> New in version 5.3.0.

5.5.12.4 CVLS linear solver interface optional output functions

The following optional outputs are available from the CVLS modules: workspace requirements, number of calls to the Jacobian routine, number of calls to the right-hand side routine for finite-difference Jacobian or Jacobian-vector product approximation, number of linear iterations, number of linear convergence failures, number of calls to the preconditioner setup and solve routines, number of calls to the Jacobian-vector setup and product routines, and last return value from a linear solver function. Note that, where the name of an output would otherwise conflict with the name of an optional output from the main solver, a suffix (for Linear Solver) has been added (e.g. `lenrwLS`).

int **CVodeGetJac**(void *cvode_mem, *SUNMatrix* *J)

> Returns the internally stored copy of the Jacobian matrix of the ODE right-hand side function.

> **Parameters**

> - **cvode_mem** – the CVODE memory structure

> - **J** – the Jacobian matrix

> **Return values**

> - **CVLS_SUCCESS** – the output value has been successfully set

> - **CVLS_MEM_NULL** – cvode_mem was NULL

> - **CVLS_LMEM_NULL** – the linear solver interface has not been initialized

> > **Warning:** This function is provided for debugging purposes and the values in the returned matrix should not be altered.

int **CVodeGetJacTime**(void *cvode_mem, sunrealtype *t_J)

> Returns the time at which the internally stored copy of the Jacobian matrix of the ODE right-hand side function was evaluated.

> **Parameters**

> - **cvode_mem** – the CVODE memory structure

> - **t_J** – the time at which the Jacobian was evaluated

> **Return values**

- **CVLS_SUCCESS** – the output value has been successfully set

- **CVLS_MEM_NULL** – cvode_mem was NULL

- **CVLS_LMEM_NULL** – the linear solver interface has not been initialized

int **CVodeGetJacNumSteps**(void *cvode_mem, long int *nst_J)

Returns the value of the internal step counter at which the internally stored copy of the Jacobian matrix of the ODE right-hand side function was evaluated.

Parameters

- **cvode_mem** – the CVODE memory structure

- **nst_J** – the value of the internal step counter at which the Jacobian was evaluated

Return values

- **CVLS_SUCCESS** – the output value has been successfully set

- **CVLS_MEM_NULL** – cvode_mem was NULL

- **CVLS_LMEM_NULL** – the linear solver interface has not been initialized

int **CVodeGetLinWorkSpace**(void *cvode_mem, long int *lenrwLS, long int *leniwLS)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- lenrwLS – the number of realtype values in the CVLS workspace.

- leniwLS – the number of integer values in the CVLS workspace.

Return value:

- CVLS_SUCCESS – The optional output values have been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

The workspace requirements reported by this routine correspond only to memory allocated within this interface and to memory allocated by the SUNLinearSolver object attached to it. The template Jacobian matrix allocated by the user outside of CVLS is not included in this report.

The previous routines CVDlsGetWorkspace and CVSpilsGetWorkspace are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

int **CVodeGetNumJacEvals**(void *cvode_mem, long int *njevals)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- njevals – the number of calls to the Jacobian function.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

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

int **CVodeGetNumLinRhsEvals**(void *cvode_mem, long int *nfevalsLS)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nfevalsLS – the number of calls made to the user-supplied right-hand side function.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

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

The previous routines CVDlsGetNumRhsEvals and CVSpilsGetNumRhsEvals are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

int **CVodeGetNumLinIters**(void *cvode_mem, long int *nliters)

The function CVodeGetNumLinIters returns the cumulative number of linear iterations.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nliters – the current number of linear iterations.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

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

int **CVodeGetNumLinConvFails**(void *cvode_mem, long int *nlcfails)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nlcfails – the current number of linear convergence failures.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

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

int **CVodeGetNumPrecEvals**(void *cvode_mem, long int *npevals)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- npevals – the current number of calls to psetup.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

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

int **CVodeGetNumPrecSolves**(void *cvode_mem, long int *npsolves)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- npsolves – the current number of calls to psolve.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

int **CVodeGetNumJTSetupEvals**(void *cvode_mem, long int *njtsetup)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- njtsetup – the current number of calls to jtsetup.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The `cvode_mem` pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

int **CVodeGetNumJtimesEvals**(void *cvode_mem, long int *njvevals)

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

> **Arguments:**

>> - `cvode_mem` – pointer to the CVODE memory block.

>> - `njvevals` – the current number of calls to `jtimes`.

> **Return value:**

>> - CVLS_SUCCESS – The optional output value has been successfully set.

>> - CVLS_MEM_NULL – The `cvode_mem` pointer is NULL.

>> - CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

int **CVodeGetLinSolvStats**(void *cvode_mem, long int *njevals, long int *nfevalsLS, long int *nliters, long int *nlcfails, long int *npevals, long int *npsolves, long int *njtsetups, long int *njtimes)

> The function `CVodeGetLinSolvStats` returns CVODE linear solver statistics.

> **Arguments:**

>> - `cvode_mem` – pointer to the CVODE memory block.

>> - `njevals` – the current number of calls to the Jacobian function.

>> - `nfevalsLS` – the current number of calls made to the user-supplied right-hand side function by the linear solver.

>> - `nliters` – the current number of linear iterations.

>> - `nlcfails` – the current number of linear convergence failures.

>> - `npevals` – the current number of calls to `psetup`.

>> - `npsolves` – the current number of calls to `psolve`.

>> - `njtsetup` – the current number of calls to `jtsetup`.

>> - `njtimes` – the current number of calls to `jtimes`.

> **Return value:**

>> - CVLS_SUCCESS – The optional output value has been successfully set.

>> - CVLS_MEM_NULL – The `cvode_mem` pointer is NULL.

>> - CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

int **CVodeGetLastLinFlag**(void *cvode_mem, long int *lsflag)

> The function `CVodeGetLastLinFlag` returns the last return value from a CVLS routine.

> **Arguments:**

>> - `cvode_mem` – pointer to the CVODE memory block.

>> - `lsflag` – the value of the last return flag from a CVLS function.

> **Return value:**

>> - CVLS_SUCCESS – The optional output value has been successfully set.

>> - CVLS_MEM_NULL – The `cvode_mem` pointer is NULL.

- CVLS_LMEM_NULL – The CVLS linear solver has not been initialized.

Notes:

If the CVLS setup function failed (i.e., *CVode()* returned CV_LSETUP_FAIL) when using the SUNLINSOL_-DENSE or SUNLINSOL_BAND modules, then the value of lsflag is equal to the column index (numbered from one) at which a zero diagonal element was encountered during the LU factorization of the (dense or banded) Jacobian matrix.

If the CVLS setup function failed when using another SUNLinearSolver module, then lsflag will be SUNLS_PSET_FAIL_UNREC, SUNLS_ASET_FAIL_UNREC, or SUNLS_PACKAGE_FAIL_UNREC.

If the CVLS solve function failed (i.e., *CVode()* returned CV_LSOLVE_FAIL), then lsflag contains the error return flag from the SUNLinearSolver object, which will be one of: SUNLS_MEM_NULL, indicating that the SUNLinearSolver memory is NULL; SUNLS_ATIMES_FAIL_UNREC, indicating an unrecoverable failure in the Jv function; SUNLS_PSOLVE_FAIL_UNREC, indicating that the preconditioner solve function psolve failed unrecoverably; SUNLS_GS_FAIL, indicating a failure in the Gram-Schmidt procedure (SPGMR and SPFGMR only); SUNLS_QRSOL_FAIL, indicating that the matrix R was found to be singular during the QR solve phase (SPGMR and SPFGMR only); or SUNLS_PACKAGE_FAIL_UNREC, indicating an unrecoverable failure in an external iterative linear solver package.

The previous routines CVDlsGetLastFlag and CVSpilsGetLastFlag are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

int **CVodeGetLinReturnFlagName**(long int lsflag)

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

Arguments:

- lsflag – a return flag from a CVLS function.

Return value:

- The return value is a string containing the name of the corresponding constant. If $1 \leq$ lsflag $\leq N$ (LU factorization failed), this routine returns "NONE".

Notes:

The previous routines CVDlsGetReturnFlagName and CVSpilsGetReturnFlagName are now wrappers for this routine, and may still be used for backward-compatibility. However, these will be deprecated in future releases, so we recommend that users transition to the new routine name soon.

5.5.12.5 Diagonal linear solver interface optional output functions

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

int **CVDiagGetWorkSpace**(void *cvode_mem, long int *lenrwLS, long int *leniwLS)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- lenrwLS – the number of realtype values in the CVDIAG workspace.

- leniwLS – the number of integer values in the CVDIAG workspace.

Return value:

- CVDIAG_SUCCESS – The optional output valus have been successfully set.

- CVDIAG_MEM_NULL – The cvode_mem pointer is NULL.

- CVDIAG_LMEM_NULL – The CVDIAG linear solver has not been initialized.

Notes:

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

int **CVDiagGetNumRhsEvals**(void *cvode_mem, long int *nfevalsLS)

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 – pointer to the CVODE memory block.

- nfevalsLS – the number of calls made to the user-supplied right-hand side function.

Return value:

- 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()*).

int **CVDiagGetLastFlag**(void *cvode_mem, long int *lsflag)

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

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- lsflag – the value of the last return flag from a CVDIAG function.

Return value:

- 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).

char ***CVDiagGetReturnFlagName**(long int lsflag)

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

Arguments:

- lsflag – a return flag from a CVDIAG function.

Return value:

- A string containing the name of the corresponding constant.

5.5.13 CVODE reinitialization function

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

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

If there are changes to the linear solver specifications, make the appropriate calls to either the linear solver objects themselves, or to the CVLS interface routines, as described in §5.5.5. Otherwise, all solver inputs set previously remain in effect.

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

int **CVodeReInit**(void *cvode_mem, *realtype* t0, *N_Vector* y0)

    The function `CVodeReInit` provides required problem specifications and reinitializes CVODE.

    Arguments:

- `cvode_mem` – pointer to the CVODE memory block.
- `t0` – is the initial value of t.
- `y0` – is the initial value of y.

    Return value:

- `CV_SUCCESS` – The call was successful.
- `CV_MEM_NULL` – The CVODE memory block was not initialized through a previous call to *CVodeCreate()*.
- `CV_NO_MALLOC` – Memory space for the CVODE memory block was not allocated through a previous call to *CVodeInit()*.
- `CV_ILL_INPUT` – An input argument was an illegal value.

    Notes:

        All previously set options are retained but may be updated by calling the appropriate "Set" functions.

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

5.6 User-supplied functions

The user-supplied functions consist of one function defining the ODE, (optionally) a function that handles error and warning messages, (optionally) a function that provides the error weight vector, (optionally) one or two functions that provide Jacobian-related information for the linear solver, and (optionally) one or two functions that define the preconditioner for use in any of the Krylov iterative algorithms.

5.6.1 ODE right-hand side

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

typedef int (*__CVRhsFn__)(*realtype* t, *N_Vector* y, *N_Vector* ydot, void *user_data);

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

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

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

> **Notes:**
>
>> Allocation of memory for ydot is handled within CVODE.
>>
>> A recoverable failure error return from the CVRhsFn is typically used to flag a value of the dependent variable y that is "illegal" in some way (e.g., negative where only a non-negative value is physically meaningful). If such a return is made, CVODE will attempt to recover (possibly repeating the nonlinear solve, or reducing the step size) in order to avoid this recoverable error return.
>>
>> For efficiency reasons, the right-hand side function is not evaluated at the converged solution of the nonlinear solver. Therefore, in general, a recoverable error in that converged value cannot be corrected. (It may be detected when the right-hand side function is called the first time during the following integration step, but a successful step cannot be undone.)
>>
>> There are two other situations in which recovery is not possible even if the right-hand side function returns a recoverable error flag. One is when this occurs at the very first call to the CVRhsFn (in which case CVODE returns CV_FIRST_RHSFUNC_ERR). The other is when a recoverable error is reported by CVRhsFn after an error test failure, while the linear multistep method order is equal to 1 (in which case CVODE returns CV_UNREC_RHSFUNC_ERR).

5.6.2 Error message handler function

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

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

> This function processes error and warning message from CVODE and it sub-modules.

> **Arguments:**

>> - `error_code` is the error code.

>> - `module` is the name of the CVODE module reporting the error.

>> - `function` is the name of the function in which the error occurred.

>> - `msg` is the error message.

>> - `eh_data` is a pointer to user data, the same as the `eh_data` parameter passed to *CVodeSetErrHandlerFn()*.

> **Return value:**

>> - void

> **Notes:**
>> `error_code` is negative for errors and positive (`CV_WARNING`) for warnings. If a function that returns a pointer to memory encounters an error, it sets `error_code` to 0.

5.6.3 Monitor function

A user may provide a function of type `CVMonitorFn` to monitor the integrator progress throughout a simulation. For example, a user may want to check integrator statistics as a simulation progresses.

typedef void (***CVMonitorFn**)(void *cvode_mem, void *user_data);

> This function is used to monitor the CVODE integrator throughout a simulation.

> **Arguments:**

>> - `cvode_mem` – the CVODE memory pointer.

>> - `user_data` – a pointer to user data, the same as the `user_data` parameter passed to *CVodeSetUserData()*.

> **Return value:**
>> Should return 0 if successful, or a negative value if unsuccessful.

> **Warning:** This function should only be utilized for monitoring the integrator progress (i.e., for debugging).

5.6.4 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 containing the weights in the WRMS norm

$$\| v \|_{\text{WRMS}} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (W_i \cdot v_i)^2}.$$

These weights will be used in place of those defined by Eq. (2.6). The function type is defined as follows:

typedef int (*__CVEwtFn__)(*N_Vector* y, *N_Vector* ewt, void *user_data);

This function computes the WRMS error weights for the vector y.

Arguments:

- y – the value of the dependent variable vector at which the weight vector is to be computed.

- ewt – the output vector containing the error weights.

- user_data a pointer to user data, the same as the user_data parameter passed to *CVodeSetUser-Data()*.

Return value:

Should return 0 if successful, or -1 if unsuccessful.

Notes:

Allocation of memory for ewt is handled within CVODE.

> **Warning:** The error weight vector must have all components positive. It is the user's responsiblity to perform this test and return -1 if it is not satisfied.

5.6.5 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:

typedef int (*__CVRootFn__)(*realtype* t, *N_Vector* y, *realtype* *gout, void *user_data);

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

Arguments:

- t – the current value of the independent variable.

- y – the current value of the dependent variable vector, $y(t)$.

- gout – the output array of length nrtfn with components $g_i(t, y)$.

- user_data a pointer to user data, the same as the user_data parameter passed to *CVodeSetUser-Data()*.

Return value:

A CVRootFn should return 0 if successful or a non-zero value if an error occured (in which case the integration is haled and CVode returns CV_RTFUNC_FAIL.

Notes:

Allocation of memory for gout is automatically handled within CVODE.

5.6.6 Projection function

When solving an IVP with a constraint equation and providing a user-defined projection operation the projection function must have type `CVProjFn`, defined as follows:

typedef int (*`CVProjFn`)(*realtype* t, *N_Vector* ycur, *N_Vector* corr, *realtype* epsProj, *N_Vector* err, void *user_data);

This function computes the projection of the solution and, if enabled, the error on to the constraint manifold.

Arguments:

- `t` – the current value of the independent variable.

- `ycur` – the current value of the dependent variable vector $y(t)$.

- `corr` – the correction, c, to the dependent variable vector so that $y(t) + c$ satisfies the constraint equation.

- `epsProj` – the tolerance to use in the nonlinear solver stopping test when solving the nonlinear constrained least squares problem.

- `err` – is on input the current error estimate, if error projection is enabled (the default) then this should be overwritten with the projected error on output. If error projection is disabled then `err` is NULL.

- `user_data` a pointer to user data, the same as the `user_data` parameter passed to *CVodeSetUser-Data()*.

Return value:
Should return 0 if successful, a negative value if an unrecoverable error occurred (the integration is halted), or a positive value if a recoverable error occurred (the integrator will, in most cases, try to correct and reattempt the step).

Notes:
The tolerance passed to the projection function (`epsProj`) is the tolerance on the iteration update in the WRMS norm, i.e., the solve should stop when the WRMS norm of the current iterate update is less than `epsProj`.

If needed by the user's projection routine, the error weight vector can be accessed by calling *CVodeGetEr-rWeights()*, and the unit roundoff is available as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

New in version 5.3.0.

5.6.7 Jacobian construction (matrix-based linear solvers)

If a matrix-based linear solver module is used (i.e., a non-NULL `SUNMatrix` object was supplied to *CVodeSetLinear-Solver()*), the user may optionally provide a function of type `CVLsJacFn` for evaluating the Jacobian of the ODE right-hand side function (or an approximation of it). `CVLsJacFn` is defined as follows:

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

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

Arguments:

- `t` – the current value of the independent variable.

- `y` – the current value of the dependent variable vector, namely the predicted value of $y(t)$.

- `fy` – the current value of the vector $f(t, y)$.

- `Jac` – the output Jacobian matrix.

- `user_data` a pointer to user data, the same as the `user_data` parameter passed to *CVodeSetUser-Data()*.

- `tmp1, tmp2, tmp3` – are pointers to memory allocated for variables of type `N_Vector` which can be used by a CVLsJacFn function as temporary storage or work space.

Return value:

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

Notes:

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

With direct linear solvers (i.e., linear solvers with type SUNLINEARSOLVER_DIRECT), the Jacobian matrix $J(t, y)$ is zeroed out prior to calling the user-supplied Jacobian function so only nonzero elements need to be loaded into `Jac`.

With the default nonlinear solver (the native SUNDIALS Newton method), each call to the user's CVLsJacFn function is preceded by a call to the CVRhsFn user function with the same (t,y) arguments. Thus, the Jacobian function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side. In the case of a user-supplied or external nonlinear solver, this is also true if the nonlinear system function is evaluated prior to calling the *linear solver setup function*.

If the user's CVLsJacFn function uses difference quotient approximations, then it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cv_mem` in `user_data` and then use the CVodeGet* functions described in §5.5.12. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in `sundials_types.h`.

Dense: A user-supplied dense Jacobian function must load the N by N dense matrix `Jac` with an approximation to the Jacobian matrix $J(t, y)$ at the point (t, y). The accessor macros SM_ELEMENT_D and SM_COLUMN_D allow the user to read and write dense matrix elements without making explicit references to the underlying representation of the SUNMATRIX_DENSE type. SM_ELEMENT_D(J, i, j) references the $(i, j$-th) element of the dense matrix `Jac` (with $i, j = 0 \ldots N - 1$). This macro is meant for small problems for which efficiency of access is not a major concern. Thus, in terms of the indices m and n ranging from 1 to N, the Jacobian element $J_{m,n}$ can be set using the statement SM_ELEMENT_D(J, m-1, n-1) = $J_{m,n}$. Alternatively, SM_COLUMN_D(J, j) returns a pointer to the first element of the j-th column of `Jac` (with $j = 0 \ldots N - 1$), and the elements of the j-th column can then be accessed using ordinary array indexing. Consequently, $J(m, n)$ can be loaded using the statements col_n = SM_COLUMN_D(J, n-1); col_n[m-1] = $J(m, n)$. For large problems, it is more efficient to use SM_COLUMN_D than to use SM_ELEMENT_D. Note that both of these macros number rows and columns starting from 0. The SUNMATRIX_DENSE type and accessor macros are documented in §7.3.

Banded: A user-supplied banded Jacobian function must load the N by N banded matrix `Jac` with the elements of the Jacobian $J(t, y)$ at the point (t, y). The accessor macros SM_ELEMENT_B, SM_COLUMN_B, and SM_COLUMN_ELEMENT_B allow the user to read and write band matrix elements without making specific references to the underlying representation of the SUNMATRIX_BAND type. SM_ELEMENT_B(J, i, j) references the (i, j), element of the band matrix `Jac`, counting from 0. This macro is meant for use in small problems for which efficiency of access is not a major concern. Thus, in terms of the indices m and n ranging from 1 to N with (m, n) within the band defined by `mupper` and `mlower`, the Jacobian element $J(m, n)$ can be loaded using the statement SM_ELEMENT_B(J, m-1, n-1) = $J(m, n)$. The elements within the band are those with -mupper $\leq m - n \leq$ mlower. Alternatively, SM_COLUMN_B(J, j) returns a pointer to the diagonal element of the j-th column of `Jac`, and if we assign this address to `realtype *col_j`, then the i-th element of the j-th column is given by SM_COLUMN_ELEMENT_B(col_j, i, j), counting from 0. Thus, for (m, n) within the band, $J(m, n)$ can be loaded by setting col_n = SM_-

COLUMN_B(J, n-1); SM_COLUMN_ELEMENT_B(col_n, m-1, n-1) = $J(m,n)$. The elements of the j-th column can also be accessed via ordinary array indexing, but this approach requires knowledge of the underlying storage for a band matrix of type SUNMATRIX_BAND. The array col_n can be indexed from -mupper to mlower. For large problems, it is more efficient to use SM_COLUMN_B and SM_COLUMN_- ELEMENT_B than to use the SM_ELEMENT_B macro. As in the dense case, these macros all number rows and columns starting from 0. The SUNMATRIX_BAND type and accessor macros are documented in §7.6.

Sparse: A user-supplied sparse Jacobian function must load the N by N compressed-sparse-column or compressed-sparse-row matrix Jac with an approximation to the Jacobian matrix $J(t,y)$ at the point (t,y). Storage for Jac already exists on entry to this function, although the user should ensure that sufficient space is allocated in Jac to hold the nonzero values to be set; if the existing space is insufficient the user may reallocate the data and index arrays as needed. The amount of allocated space in a SUNMATRIX_- SPARSE object may be accessed using the macro SM_NNZ_S or the routine SUNSparseMatrix_NNZ. The SUNMATRIX_SPARSE type and accessor macros are documented in §7.8.

The previous function type CVDlsJacFn is identical to *CVLsJacFn*, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

5.6.8 Linear system construction (matrix-based linear solvers)

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

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

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

Arguments:

- t – the current value of the independent variable.

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

- fy – the current value of the vector $f(t,y)$.

- M – the output linear system matrix.

- jok – an input flag indicating whether the Jacobian-related data needs to be updated. The jok flag enables reusing of Jacobian data across linear solves however, the user is responsible for storing Jacobian data for reuse. jok = SUNFALSE means that the Jacobian-related data must be recomputed from scratch. jok = SUNTRUE means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of γ). A call with jok = SUNTRUE can only occur after a call with jok = SUNFALSE.

- jcur – a pointer to a flag which should be set to SUNTRUE if Jacobian data was recomputed, or set to SUNFALSE if Jacobian data was not recomputed, but saved data was still reused.

- gamma – the scalar γ appearing in the matrix $M = I - \gamma J$.

- user_data – a pointer to user data, the same as the user_data parameter passed to *CVodeSetUser-Data()*.

- tmp1, tmp2, tmp3 – are pointers to memory allocated for variables of type N_Vector which can be used by a CVLsLinSysFn function as temporary storage or work space.

Return value:
Should return 0 if successful, a positive value if a recoverable error occurred (in which case CVODE will attempt to correct, while CVLS sets last_flag to CVLS_JACFUNC_RECVR), or a negative value if it failed

unrecoverably (in which case the integration is halted, *CVode()* returns CV_LSETUP_FAIL and CVLS sets last_flag to CVLS_JACFUNC_UNRECVR).

5.6.9 Jacobian-vector product (matrix-free linear solvers)

If a matrix-free linear solver is to be used (i.e., a NULL-valued SUNMATRIX was supplied to *CVodeSetLinear-Solver()*, the user may provide a function of type *CVLsJacTimesVecFn* in the following form, to compute matrix-vector products Jv. If such a function is not supplied, the default is a difference quotient approximation to these products.

typedef int (****CVLsJacTimesVecFn**)(*N_Vector* v, *N_Vector* Jv, *realtype* t, *N_Vector* y, *N_Vector* fy, void *user_data, *N_Vector* tmp);

> This function computes the product $Jv = \dfrac{\partial f(t, y)}{\partial y} v$ (or an approximation to it).
>
> **Arguments:**
>> - v – the vector by which the Jacobian must be multiplied.
>>
>> - Jv – the output vector computed.
>>
>> - t – the current value of the independent variable.
>>
>> - y – the current value of the dependent variable vector.
>>
>> - fy – the current value of the vector $f(t, y)$.
>>
>> - user_data – a pointer to user data, the same as the user_data parameter passed to *CVodeSetUserData()*.
>>
>> - tmp – a pointer to memory allocated for a variable of type N_Vector which can be used for work space.
>
> **Return value:**
>> The value returned by the Jacobian-vector product function should be 0 if successful. Any other return value will result in an unrecoverable error of the generic Krylov solver, in which case the integration is halted.
>
> **Notes:**
>> This function must return a value of Jv that uses the *current* value of J, i.e. as evaluated at the current (t, y).
>>
>> If the user's *CVLsJacTimesVecFn* function uses difference quotient approximations, it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to cvode_mem to user_data and then use the CVodeGet* functions described in §5.5.12.1. The unit roundoff can be accessed as UNIT_-ROUNDOFF defined in sundials_types.h.
>>
>> The previous function type CVSpilsJacTimesVecFn is identical to *CVLsJacTimesVecFn()*, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

5.6.10 Jacobian-vector product setup (matrix-free linear solvers)

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

typedef int (***CVLsJacTimesSetupFn**)(*realtype* t, *N_Vector* y, *N_Vector* fy, void *user_data);

> This function preprocesses and/or evaluates Jacobian-related data needed by the Jacobian-times-vector routine.

> **Arguments:**
>
> > - t – the current value of the independent variable.
> >
> > - y – the current value of the dependent variable vector.
> >
> > - fy – the current value of the vector $f(t, y)$.
> >
> > - user_data – a pointer to user data, the same as the user_data parameter passed to *CVodeSetUser-Data()*.

> **Return value:**
> > The value returned by the Jacobian-vector setup function should be 0 if successful, positive for a recoverable error (in which case the step will be retried), or negative for an unrecoverable error (in which case the integration is halted).

> **Notes:**
> > Each call to the Jacobian-vector setup function is preceded by a call to the *CVRhsFn* user function with the same (t, y) arguments. Thus, the setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side.

> > If the user's CVLsJacTimesSetupFn function uses difference quotient approximations, it may need to access quantities not in the argument list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to cvode_mem to user_data and then use the CVodeGet* functions described in §5.5.12.1. The unit roundoff can be accessed as UNIT_ROUNDOFF defined in sundials_types.h.

> > The previous function type CVSpilsJacTimesSetupFn is identical to *CVLsJacTimesSetupFn*, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

5.6.11 Preconditioner solve (iterative linear solvers)

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

typedef int (***CVLsPrecSolveFn**)(*realtype* t, *N_Vector* y, *N_Vector* fy, *N_Vector* r, *N_Vector* z, *realtype* gamma,
realtype delta, int lr, void *user_data);

> This function solves the preconditioned system $Pz = r$.

> **Arguments:**
>
> > - t – the current value of the independent variable.
> >
> > - y – the current value of the dependent variable vector.
> >
> > - fy – the current value of the vector $f(t, y)$.
> >
> > - r – the right-hand side vector of the linear system.

- `z` – the computed output vector.

- `gamma` – the scalar $gamma$ in the matrix given by $M = I - \gamma J$.

- `delta` – an input tolerance to be used if an iterative method is employed in the solution. In that case, the residual vector $Res = r - Pz$ of the system should be made less than `delta` in the weighted l_2 norm, i.e., $\sqrt{\sum_i (Res_i \cdot ewt_i)^2} < $ `delta`. To obtain the `N_Vector ewt`, call *CVodeGetErrWeights()*.

- `lr` – an input flag indicating whether the preconditioner solve function is to use the left preconditioner (`lr = 1`) or the right preconditioner (`lr = 2`).

- `user_data` – a pointer to user data, the same as the `user_data` parameter passed to *CVodeSetUser-Data()*.

Return value:

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

Notes:

The previous function type CVSpilsPrecSolveFn is identical to *CVLsPrecSolveFn*, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

5.6.12 Preconditioner setup (iterative linear solvers)

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

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

This function preprocesses and/or evaluates Jacobian-related data needed by the preconditioner.

Arguments:

- `t` – the current value of the independent variable.

- `y` – the current value of the dependent variable vector, namely the predicted value of $y(t)$.

- `fy` – the current value of the vector $f(t, y)$.

- `jok` – an input flag indicating whether the Jacobian-related data needs to be updated. The `jok` argument provides for the reuse of Jacobian data in the preconditioner solve function. `jok = SUNFALSE` means that the Jacobian-related data must be recomputed from scratch. `jok = SUNTRUE` means that the Jacobian data, if saved from the previous call to this function, can be reused (with the current value of γ). A call with `jok = SUNTRUE` can only occur after a call with `jok = SUNFALSE`.

- `jcur` – a pointer to a flag which should be set to `SUNTRUE` if Jacobian data was recomputed, or set to `SUNFALSE` if Jacobian data was not recomputed, but saved data was still reused.

- `gamma` – the scalar γ appearing in the matrix $M = I - \gamma J$.

- `user_data` – a pointer to user data, the same as the `user_data` parameter passed to *CVodeSetUser-Data()*.

Return value:

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

Notes:

The operations performed by this function might include forming a crude approximate Jacobian and performing an LU factorization of the resulting approximation to $M = I - \gamma J$.

With the default nonlinear solver (the native SUNDIALS Newton method), each call to the preconditioner setup function is preceded by a call to the *CVRhsFn* user function with the same (t, y) arguments. Thus, the preconditioner setup function can use any auxiliary data that is computed and saved during the evaluation of the ODE right-hand side. In the case of a user-supplied or external nonlinear solver, this is also true if the nonlinear system function is evaluated prior to calling the linear solver setup function (see §9.1.4 for more information).

This function is not called in advance of every call to the preconditioner solve function, but rather is called only as often as needed to achieve convergence in the nonlinear solver.

If the user's `CVLsPrecSetupFn` function uses difference quotient approximations, it may need to access quantities not in the call list. These include the current step size, the error weights, etc. To obtain these, the user will need to add a pointer to `cvode_mem` to `user_data` and then use the `CVodeGet*` functions described in §5.5.12. The unit roundoff can be accessed as `UNIT_ROUNDOFF` defined in `sundials_types.h`.

The previous function type `CVSpilsPrecSetupFn` is identical to *CVLsPrecSetupFn*, and may still be used for backward-compatibility. However, this will be deprecated in future releases, so we recommend that users transition to the new function type name soon.

5.7 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.

5.7.1 A serial banded preconditioner module

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

In order to use the CVBANDPRE module, the user need not define any additional functions. Aside from the header files required for the integration of the ODE problem (see §5.3), 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 changed from the skeleton program presented in §5.4 are shown in bold.

1. Initialize multi-threaded environment, if appropriate

2. Create the `SUNContext` object.

3. Set problem dimensions etc.

4. Set vector of initial values

5. Create CVODE object

6. Initialize CVODE solver

7. Specify integration tolerances

8. **Create linear solver object**

   When creating the iterative linear solver object, specify the type of preconditioning (`SUN_PREC_LEFT` or `SUN_PREC_RIGHT`) to use.

9. Set linear solver optional inputs

10. Attach linear solver module

11. **Initialize the CVBANDPRE preconditioner module**

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

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

    to allocate memory and initialize the internal preconditioner data.

12. Set optional inputs.

    Note that the user should not overwrite the preconditioner setup function or solve function through calls to the *CVodeSetPreconditioner()* optional input function.

13. Create nonlinear solver object

14. Attach nonlinear solver module

15. Set nonlinear solver optional inputs

16. Specify rootfinding problem

17. Advance solution in time

18. **Get optional outputs**

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

19. Deallocate memory for solution vector

20. Free solver memory

21. Free nonlinear solver memory

22. Free linear solver memory

23. Free the SUNContext object

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

int **CVBandPrecInit**(void *cvode_mem, *sunindextype* N, *sunindextype* mu, *sunindextype* ml)

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

   Arguments:

   - `cvode_mem` – pointer to the CVODE memory block.

   - `N` – problem dimension.

   - `mu` – upper half-bandwidth of the Jacobian approximation.

   - `ml` – lower half-bandwidth of the Jacobian approximation.

   Return value:

- CVLS_SUCCESS – The call to CVBandPrecInit was successful.

- CVLS_MEM_NULL – The cvode_mem pointer is NULL.

- CVLS_MEM_FAIL – A memory allocation request has failed.

- CVLS_LMEM_NULL – A CVLS linear solver memory was not attached.

- CVLS_ILL_INPUT – The supplied vector implementation was not compatible with block band precon-
  ditioner.

Notes:

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

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

int **CVBandPrecGetWorkSpace**(void *cvode_mem, long int *lenrwBP, long int *leniwBP)

The function CVBandPrecGetWorkSpace returns the sizes of the CVBANDPRE real and integer workspaces.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- lenrwBP – the number of realtype values in teh CVBANDPRE workspace.

- leniwBP – the number of integer values in the CVBANDPRE workspace.

Return value:

- CVLS_SUCCESS – The optional output values have been successfully set.

- CVLS_PMEM_NULL – The CVBANDPRE preconditioner has not been initialized.

Notes:

The workspace requirements reported by this routine correspond only to memory allocated within the
CVBANDPRE module (the banded matrix approximation, banded SUNLinearSolver object, and tem-
porary vectors).

The workspaces referred to here exist in addition to those given by the corresponding function
CVodeGetLinWorkSpace.

int **CVBandPrecGetNumRhsEvals**(void *cvode_mem, long int *nfevalsBP)

The function CVBandPrecGetNumRhsEvals returns the number of calls made to the user-supplied right-hand
side function for the finite difference banded Jacobian approximation used within the preconditioner setup func-
tion.

Arguments:

- cvode_mem – pointer to the CVODE memory block.

- nfevalsBP – the number of calls to the user right-hand side function.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_PMEM_NULL – The CVBANDPRE preconditioner has not been initialized.

Notes:

The counter nfevalsBP is distinct from the counter nfevalsLS returned by the corresponding function
CVodeGetNumLinRhsEvals() and nfevals returned by *CVodeGetNumRhsEvals()*.The total number of
right-hand side function evaluations is the sum of all three of these counters.

5.7.2 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 (2.7) 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 [39] and is included in a software module within the CVODE package. This module works with the parallel vector module NVECTOR_PARALLEL and is usable with any of the Krylov iterative linear solvers through the CVLS interface. It generates a preconditioner that is a block-diagonal matrix with each block being a band matrix. The blocks need not have the same number of super- and sub-diagonals and these numbers may vary from block to block. This Band-Block-Diagonal Preconditioner module is called CVBBDPRE.

One way to envision these preconditioners is to think of the domain of the computational PDE problem as being subdivided into M non-overlapping subdomains. Each of these subdomains is then assigned to one of the M processes to be used to solve the ODE system. The basic idea is to isolate the preconditioning so that it is local to each process, and also to use a (possibly cheaper) approximate right-hand side function. This requires the definition of a new function $g(t, y)$ which approximates the function $f(t, y)$ in the definition of the ODE system (2.1). However, the user may set $g = f$. Corresponding to the domain decomposition, there is a decomposition of the solution vector y into M disjoint blocks y_m, and a decomposition of g into blocks g_m. The block g_m depends both on y_m and on components of blocks $y_{m'}$ associated with neighboring subdomains (so-called ghost-cell data). Let $\bar{y}_m$ denote y_m augmented with those other components on which g_m depends. Then we have

$$g(t, y) = \begin{bmatrix} g_1(t, \bar{y}_1) & g_2(t, \bar{y}_2) & \cdots & g_M(t, \bar{y}_M) \end{bmatrix}^T$$

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

$$P = \begin{bmatrix} P_1 & & & \\ & P_2 & & \\ & & \ddots & \\ & & & P_M \end{bmatrix}$$

where

$$P_m \approx I - \gamma J_m$$

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

$$Px = b$$

reduces to solving each of the equations

$$P_m x_m = b_m$$

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.

typedef int (***CVLocalFn**)(*sunindextype* Nlocal, *realtype* t, *N_Vector* y, *N_Vector* glocal, void *user_data);

This `gloc` function computes $g(t, y)$. It loads the vector `glocal` as a function of `t` and `y`.

Arguments:

- `Nlocal` – the local vector length.

- `t` – the value of the independent variable.

- `y` – the dependent variable.

- `glocal` – the output vector.

- `user_data` – 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.

typedef int (***CVCommFn**)(*sunindextype* Nlocal, *realtype* t, *N_Vector* y, void *user_data);

This `cfn` function performs all interprocess communication necessary for the execution of the `gloc` function above, using the input vector `y`.

Arguments:

- `Nlocal` – the local vector length.

- `t` – the value of the independent variable.

- `y` – the dependent variable.

- `user_data` – 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 §5.3), 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 usage of this module. Steps that are changed from the skeleton program presented in §5.4 are shown in bold.

1. Initialize MPI environment

2. Create the `SUNContext` object

3. Set problem dimensions etc.

4. Set vector of initial values

5. Create CVODE object

6. Initialize CVODE solver

7. Specify integration tolerances

8. **Create linear solver object**

   When creating the iterative linear solver object, specify the type of preconditioning (`SUN_PREC_LEFT` or `SUN__PREC_RIGHT`) to use.

9. Set linear solver optional inputs

10. Attach linear solver module

11. **Initialize the CVBBDPRE preconditioner module**

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

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

    to allocate memory and initialize the internal preconditioner data. The last two arguments of *CVBBDPrecInit()* are the two user-supplied functions described above.

12. Set optional inputs

    Note that the user should not overwrite the preconditioner setup function or solve function through calls to the *CVodeSetPreconditioner()* optional input function.

13. Create nonlinear solver object

14. Attach nonlinear solver module

15. Set nonlinear solver optional inputs

16. Specify rootfinding problem

17. Advance solution in time

18. **Get optional outputs**

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

19. Deallocate memory for solution vector

20. Free solver memory

21. Free nonlinear solver memory

22. Free linear solver memory

23. Free the `SUNContext` object

24. Finalize MPI

The user-callable functions that initialize or re-initialize the CVBBDPRE preconditioner module are described next.

int **CVBBDPrecInit**(void *cvode_mem, *sunindextype* local_N, *sunindextype* mudq, *sunindextype* mldq, *sunindextype* mukeep, *sunindextype* mlkeep, *realtype* dqrely, *CVLocalFn* gloc, *CVCommFn* cfn)

> The function `CVBBDPrecInit` initializes and allocates (internal) memory for the CVBBDPRE preconditioner.

> **Arguments:**

> - `cvode_mem` – pointer to the CVODE memory block.

> - `local_N` – local vector length.

> - `mudq` – upper half-bandwidth to be used in the difference quotient Jacobian approximation.

> - `mldq` – lower half-bandwidth to be used in the difference quotient Jacobian approximation.

> - `mukeep` – upper half-bandwidth of the retained banded approximate Jacobian block.

> - `mlkeep` – lower half-bandwidth of the retained banded approximate Jacobian block.

> - `dqrely` – 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` – the *CVLocalFn* function which computes the approximation $g(t, y) \approx f(t, y)$.

> - `cfn` – the *CVCommFn* which performs all interprocess communication required for the computation of $g(t, y)$.

> **Return value:**

> - `CVLS_SUCCESS` – The function was successful

> - `CVLS_MEM_NULL` – The `cvode_mem` pointer is `NULL`.

> - `CVLS_MEM_FAIL` – A memory allocation request has failed.

> - `CVLS_LMEM_NULL` – A CVLS linear solver memory was not attached.

> - `CVLS_ILL_INPUT` – The supplied vector implementation was not compatible with block band preconditioner.

> **Notes:**

> If one of the half-bandwidths `mudq` or `mldq` to be used in the difference quotient calculation of the approximate Jacobian is negative or exceeds the value `local_N - 1 ``, it is replaced by ``0` or `local_N - 1` accordingly.

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

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

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

The CVBBDPRE module also provides a reinitialization function to allow solving a sequence of problems of the same size, with the same linear solver choice, provided there is no change in `local_N`, `mukeep`, or `mlkeep`. After solving one problem, and after calling *CVodeReInit()* to re-initialize CVODE for a subsequent problem, a call to *CVBBDPrecReInit()* can be made to change any of the following: the half-bandwidths `mudq` and `mldq` used in the difference-quotient Jacobian approximations, the relative increment `dqrely`, or one of the user-supplied functions `gloc` and `cfn`. If there is a change in any of the linear solver inputs, an additional call to the "set" routines provided by the

SUNLinearSolver module, and/or one or more of the corresponding CVLS "set" functions, must also be made (in the proper order).

int **CVBBDPrecReInit**(void *cvode_mem, *sunindextype* mudq, *sunindextype* mldq, *realtype* dqrely)

> The function CVBBDPrecReInit re-initializes the CVBBDPRE preconditioner.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * mudq – upper half-bandwidth to be used in the difference quotient Jacobian approximation.
> >
> > * mldq – lower half-bandwidth to be used in the difference quotient Jacobian approximation.
> >
> > * dqrely – the relative increment in components of
>
> **Return value:**
>
> > * CVLS_SUCCESS – The function was successful
> >
> > * CVLS_MEM_NULL – The cvode_mem pointer is NULL. cvode_mem pointer was NULL.
> >
> > * CVLS_LMEM_NULL – A CVLS linear solver memory was not attached.
> >
> > * CVLS_PMEM_NULL – The function *CVBBDPrecInit()* was not previously called
>
> **Notes:**
> > If one of the half-bandwidths mudq or mldq is negative or exceeds the value local_N-1, it is replaced by 0 or local_N-1 accordingly.

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

int **CVBBDPrecGetWorkSpace**(void *cvode_mem, long int *lenrwBBDP, long int *leniwBBDP)

> The function CVBBDPrecGetWorkSpace returns the local CVBBDPRE real and integer workspace sizes.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * lenrwBBDP – local number of realtype values in the CVBBDPRE workspace.
> >
> > * leniwBBDP – local number of integer values in the CVBBDPRE workspace.
>
> **Return value:**
>
> > * CVLS_SUCCESS – The optional output value has been successfully set.
> >
> > * CVLS_MEM_NULL – The cvode_mem pointer was NULL.
> >
> > * CVLS_PMEM_NULL – The CVBBDPRE preconditioner has not been initialized.
>
> **Notes:**
> > The workspace requirements reported by this routine correspond only to memory allocated within the CVBBDPRE module (the banded matrix approximation, banded SUNLinearSolver object, temporary vectors). These values are local to each process. The workspaces referred to here exist in addition to those given by the corresponding function CVodeGetLinWorkSpace.

int **CVBBDPrecGetNumGfnEvals**(void *cvode_mem, long int *ngevalsBBDP)

> The function CVBBDPrecGetNumGfnEvals returns the number of calls made to the user-supplied gloc function due to the finite difference approximation of the Jacobian blocks used within the preconditioner setup function.
>
> **Arguments:**
>
> > * cvode_mem – pointer to the CVODE memory block.
> >
> > * ngevalsBBDP – the number of calls made to the user-supplied gloc function due to the finite difference approximation of the Jacobian blocks used within the preconditioner setup function.

Return value:

- CVLS_SUCCESS – The optional output value has been successfully set.

- CVLS_MEM_NULL – The cvode_mem pointer was NULL.

- CVLS_PMEM_NULL – The CVBBDPRE preconditioner has not been initialized.

In addition to the ngevalsBBDP gloc evaluations, the costs associated with CVBBDPRE also include nlinsetups LU factorizations, nlinsetups calls to cfn, npsolves banded backsolve calls, and nfevalsLS right-hand side function evaluations, where nlinsetups is an optional CVODE output and npsolves and nfevalsLS are linear solver optional outputs (see §5.5.12).

Chapter 6

Vector Data Structures

The SUNDIALS library comes packaged with a variety of NVECTOR implementations, designed for simulations in serial, shared-memory parallel, and distributed-memory parallel environments, as well as interfaces to vector data structures used within external linear solver libraries. All native implementations assume that the process-local data is stored contiguously, and they in turn provide a variety of standard vector algebra operations that may be performed on the data.

In addition, SUNDIALS provides a simple interface for generic vectors (akin to a C++ *abstract base class*). All of the SUNDIALS packages (CVODE(s), IDA(s), KINSOL, ARKODE) in turn are constructed to only depend on these generic vector operations, making them immediately extensible to new user-defined vector objects. The only exceptions to this rule relate to the direct linear solver modules (and associated matrices), since they rely on particular data storage and access patterns in the NVECTORS used.

6.1 Description of the NVECTOR Modules

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, and specific to, the particular NVECTOR implementation. Users can provide a custom implementation of the NVECTOR module or use one provided within SUNDIALS. 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**

and the generic structure is defined as

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

Here, the `_generic_N_Vector_Op` structure is essentially a list of function pointers to the various actual vector operations, and is defined as

```
struct _generic_N_Vector_Ops {
   N_Vector_ID  (*nvgetvectorid)(N_Vector);
```

(continues on next page)

```
N_Vector     (*nvclone)(N_Vector);
N_Vector     (*nvcloneempty)(N_Vector);
void         (*nvdestroy)(N_Vector);
void         (*nvspace)(N_Vector, sunindextype *, sunindextype *);
realtype*    (*nvgetarraypointer)(N_Vector);
realtype*    (*nvgetdevicearraypointer)(N_Vector);
void         (*nvsetarraypointer)(realtype *, N_Vector);
void*        (*nvgetcommunicator)(N_Vector);
sunindextype (*nvgetlength)(N_Vector);
sunindextype (*nvgetlocallength)(N_Vector);
void         (*nvlinearsum)(realtype, N_Vector, realtype, N_Vector, N_Vector);
void         (*nvconst)(realtype, N_Vector);
void         (*nvprod)(N_Vector, N_Vector, N_Vector);
void         (*nvdiv)(N_Vector, N_Vector, N_Vector);
void         (*nvscale)(realtype, N_Vector, N_Vector);
void         (*nvabs)(N_Vector, N_Vector);
void         (*nvinv)(N_Vector, N_Vector);
void         (*nvaddconst)(N_Vector, realtype, N_Vector);
realtype     (*nvdotprod)(N_Vector, N_Vector);
realtype     (*nvmaxnorm)(N_Vector);
realtype     (*nvwrmsnorm)(N_Vector, N_Vector);
realtype     (*nvwrmsnormmask)(N_Vector, N_Vector, N_Vector);
realtype     (*nvmin)(N_Vector);
realtype     (*nvwl2norm)(N_Vector, N_Vector);
realtype     (*nvl1norm)(N_Vector);
void         (*nvcompare)(realtype, N_Vector, N_Vector);
booleantype  (*nvinvtest)(N_Vector, N_Vector);
booleantype  (*nvconstrmask)(N_Vector, N_Vector, N_Vector);
realtype     (*nvminquotient)(N_Vector, N_Vector);
int          (*nvlinearcombination)(int, realtype *, N_Vector *, N_Vector);
int          (*nvscaleaddmulti)(int, realtype *, N_Vector, N_Vector *, N_Vector *);
int          (*nvdotprodmulti)(int, N_Vector, N_Vector *,  realtype *);
int          (*nvlinearsumvectorarray)(int, realtype, N_Vector *, realtype,
                                       N_Vector *, N_Vector *);
int          (*nvscalevectorarray)(int, realtype *,  N_Vector *, N_Vector *);
int          (*nvconstvectorarray)(int, realtype, N_Vector *);
int          (*nvwrmsnomrvectorarray)(int, N_Vector *, N_Vector *, realtype *);
int          (*nvwrmsnomrmaskvectorarray)(int, N_Vector *, N_Vector *, N_Vector,
                                          realtype *);
int          (*nvscaleaddmultivectorarray)(int, int, realtype *, N_Vector *,
                                           N_Vector **, N_Vector **);
int          (*nvlinearcombinationvectorarray)(int, int, realtype *, N_Vector **,
                                               N_Vector *);
realtype     (*nvdotprodlocal)(N_Vector, N_Vector);
realtype     (*nvmaxnormlocal)(N_Vector);
realtype     (*nvminlocal)(N_Vector);
realtype     (*nvl1normlocal)(N_Vector);
booleantype  (*nvinvtestlocal)(N_Vector, N_Vector);
booleantype  (*nvconstrmasklocal)(N_Vector, N_Vector, N_Vector);
realtype     (*nvminquotientlocal)(N_Vector, N_Vector);
realtype     (*nvwsqrsumlocal)(N_Vector, N_Vector);
realtype     (*nvwsqrsummasklocal(N_Vector, N_Vector, N_Vector);
```

```
    int         (*nvdotprodmultilocal)(int, N_Vector, N_Vector *, realtype *);
    int         (*nvdotprodmultiallreduce)(int, N_Vector, realtype *);
    int         (*nvbufsize)(N_Vector, sunindextype *);
    int         (*nvbufpack)(N_Vector, void*);
    int         (*nvbufunpack)(N_Vector, void*);
};
```

The generic NVECTOR module defines and implements the vector operations acting on a `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 operation $z \leftarrow cx$ for vectors x and z and a scalar c:

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

§6.2 contains a complete list of all standard vector operations defined by the generic NVECTOR module. §6.2.2, §6.2.3, §6.2.4, §6.2.5, and §6.2.6 list *optional* fused, vector array, local reduction, single buffer reduction, and exchange operations, respectively.

Fused and vector array operations (see §6.2.2 and §6.2.3) are intended to increase data reuse, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. If a particular NVECTOR implementation defines a fused or vector array operation as `NULL`, the generic NVECTOR module will automatically call standard vector operations as necessary to complete the desired operation. In all SUNDIALS-provided NVECTOR implementations, all fused and vector array operations are disabled by default. However, these implementations provide additional user-callable functions to enable/disable any or all of the fused and vector array operations. See the following sections for the implementation specific functions to enable/disable operations.

Local reduction operations (see §6.2.4) are similarly intended to reduce parallel communication on distributed memory systems, particularly when NVECTOR objects are combined together within an NVECTOR_MANYVECTOR object (see §6.17). If a particular NVECTOR implementation defines a local reduction operation as `NULL`, the NVECTOR_-MANYVECTOR module will automatically call standard vector reduction operations as necessary to complete the desired operation. All SUNDIALS-provided NVECTOR implementations include these local reduction operations, which may be used as templates for user-defined implementations.

The single buffer reduction operations (§6.2.5) are used in low-synchronization methods to combine separate reductions into one `MPI_Allreduce` call.

The exchange operations (see §6.2.6) are intended only for use with the XBraid library for parallel-in-time integration (accessible from ARKODE) and are otherwise unused by SUNDIALS packages.

6.1.1 NVECTOR Utility Functions

The generic NVECTOR module also defines several utility functions to aid in creation and management of arrays of `N_Vector` objects – these functions are particularly useful for Fortran users to utilize the NVECTOR_MANYVECTOR or SUNDIALS' sensitivity-enabled packages CVODES and IDAS.

The functions *N_VCloneVectorArray()* and *N_VCloneVectorArrayEmpty()* create (by cloning) an array of *count* variables of type *N_Vector*, each of the same type as an existing `N_Vector` input:

N_Vector *__N_VCloneVectorArray__*(int count, *N_Vector* w)

Clones an array of `count` N_Vector objects, allocating their data arrays (similar to *N_VClone()*).

Arguments:

- count – number of N_Vector objects to create.

- w – template *N_Vector* to clone.

Return value:

- pointer to a new N_Vector array on success.

- NULL pointer on failure.

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

Clones an array of count N_Vector objects, leaving their data arrays unallocated (similar to *N_-VCloneEmpty()*).

Arguments:

- count – number of N_Vector objects to create.

- w – template *N_Vector* to clone.

Return value:

- pointer to a new N_Vector array on success.

- NULL pointer on failure.

An array of variables of type *N_Vector* can be destroyed by calling *N_VDestroyVectorArray()*:

void **N_VDestroyVectorArray**(*N_Vector* *vs, int count)

Destroys an array of count N_Vector objects.

Arguments:

- vs – N_Vector array to destroy.

- count – number of N_Vector objects in vs array.

Notes:

This routine will internally call the N_Vector implementation-specific *N_VDestroy()* operation.

If vs was allocated using *N_VCloneVectorArray()* then the data arrays for each N_Vector object will be freed; if vs was allocated using *N_VCloneVectorArrayEmpty()* then it is the user's responsibility to free the data for each N_Vector object.

Finally, we note that users of the Fortran 2003 interface may be interested in the additional utility functions *N_VNewVectorArray()*, *N_VGetVecAtIndexVectorArray()*, and *N_VSetVecAtIndexVectorArray()*, that are wrapped as FN_NewVectorArray, FN_VGetVecAtIndexVectorArray, and FN_VSetVecAtIndexVectorArray, respectively. These functions allow a Fortran 2003 user to create an empty vector array, access a vector from this array, and set a vector within this array:

N_Vector ***N_VNewVectorArray**(int count)

Creates an array of count N_Vector objects, the pointers to each are initialized as NULL.

Arguments:

- count – length of desired N_Vector array.

Return value:

- pointer to a new N_Vector array on success.

- NULL pointer on failure.

N_Vector ***N_VGetVecAtIndexVectorArray**(*N_Vector* *vs, int index)

>   Accesses the N_Vector at the location index within the N_Vector array vs.

>   **Arguments:**

>>   - vs – N_Vector array.

>>   - index – desired N_Vector to access from within vs.

>   **Return value:**

>>   - pointer to the indexed N_Vector on success.

>>   - NULL pointer on failure (index < 0 or vs == NULL).

>   **Notes:**

>>   This routine does not verify that index is within the extent of vs, since vs is a simple N_Vector array that does not internally store its allocated length.

void **N_VSetVecAtIndexVectorArray**(*N_Vector* *vs, int index, *N_Vector* w)

>   Sets a pointer to w at the location index within the vector array vs.

>   **Arguments:**

>>   - vs – N_Vector array.

>>   - index – desired location to place the pointer to w within vs.

>>   - w – N_Vector to set within vs.

>   **Notes:**

>>   This routine does not verify that index is within the extent of vs, since vs is a simple N_Vector array that does not internally store its allocated length.

6.1.2 Implementing a custom NVECTOR

A particular implementation of the NVECTOR module must:

- Specify the *content* field of the N_Vector structure.

- 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.

To aid in the creation of custom NVECTOR modules, the generic NVECTOR module provides two utility functions *N_-VNewEmpty()* and *N_VCopyOps()*. When used in custom NVECTOR constructors and clone routines these functions will ease the introduction of any new optional vector operations to the NVECTOR API by ensuring that only required operations need to be set, and that all operations are copied when cloning a vector.

N_Vector **N_VNewEmpty**()

>   This allocates a new generic N_Vector object and initializes its content pointer and the function pointers in the operations structure to NULL.

Return value: If successful, this function returns an `N_Vector` object. If an error occurs when allocating the object, then this routine will return `NULL`.

void **N_VFreeEmpty**(*N_Vector* v)

This routine frees the generic `N_Vector` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments:

- *v* – an N_Vector object

int **N_VCopyOps**(*N_Vector* w, *N_Vector* v)

This function copies the function pointers in the `ops` structure of `w` into the `ops` structure of `v`.

Arguments:

- *w* – the vector to copy operations from

- *v* – the vector to copy operations to

Return value: If successful, this function returns `0`. If either of the inputs are `NULL` or the `ops` structure of either input is `NULL`, then is function returns a non-zero value.

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	*hypre* ParHyp parallel vector	4
SUNDIALS_NVEC_PETSC	PETSc parallel vector	5
SUNDIALS_NVEC_CUDA	CUDA vector	6
SUNDIALS_NVEC_HIP	HIP vector	7
SUNDIALS_NVEC_SYCL	SYCL vector	8
SUNDIALS_NVEC_RAJA	RAJA vector	9
SUNDIALS_NVEC_OPENMPDEV	OpenMP vector with device offloading	10
SUNDIALS_NVEC_TRILINOS	Trilinos Tpetra vector	11
SUNDIALS_NVEC_MANYVECTOR	"ManyVector" vector	12
SUNDIALS_NVEC_MPIMANYVECTOR	MPI-enabled "ManyVector" vector	13
SUNDIALS_NVEC_MPIPLUSX	MPI+X vector	14
SUNDIALS_NVEC_CUSTOM	User-provided custom vector	15

6.1.3 Support for complex-valued vectors

While SUNDIALS itself is written under an assumption of real-valued data, it does provide limited support for complex-valued problems. However, since none of the built-in NVECTOR modules supports complex-valued data, users must provide a custom NVECTOR implementation for this task. Many of the NVECTOR routines described in the subsection §6.2 naturally extend to complex-valued vectors; however, some do not. To this end, we provide the following guidance:

- `N_VMin()` and `N_VMinLocal()` should return the minimum of all *real* components of the vector, i.e., $m = \min_{0 \le i < n} \text{real}(x_i)$.

- `N_VConst()` (and similarly `N_VConstVectorArray()`) should set the real components of the vector to the input constant, and set all imaginary components to zero, i.e., $z_i = c + 0j$ for $0 \le i < n$.

- `N_VAddConst()` should only update the real components of the vector with the input constant, leaving all imaginary components unchanged.

- `N_VWrmsNorm()`, `N_VWrmsNormMask()`, `N_VWSqrSumLocal()` and `N_VWSqrSumMaskLocal()` should assume that all entries of the weight vector `w` and the mask vector `id` are real-valued.

- `N_VDotProd()` should mathematically return a complex number for complex-valued vectors; as this is not possible with SUNDIALS' current `realtype`, this routine should be set to `NULL` in the custom NVECTOR implementation.

- `N_VCompare()`, `N_VConstrMask()`, `N_VMinQuotient()`, `N_VConstrMaskLocal()` and `N_VMinQuotient-Local()` are ill-defined due to the lack of a clear ordering in the complex plane. These routines should be set to `NULL` in the custom NVECTOR implementation.

While many SUNDIALS solver modules may be utilized on complex-valued data, others cannot. Specifically, although each package's linear solver interface (e.g., ARKLS or CVLS) may be used on complex-valued problems, none of the built-in SUNMatrix or SUNLinearSolver modules will work (all of the direct linear solvers must store complex-valued data, and all of the iterative linear solvers require `N_VDotProd()`). Hence a complex-valued user must provide custom linear solver modules for their problem. At a minimum this will consist of a custom SUNLinearSolver implementation (see §8.1.8), and optionally a custom SUNMatrix as well. The user should then attach these modules as normal to the package's linear solver interface.

Similarly, although both the *SUNNonlinearSolver_Newton* and *SUNNonlinearSolver_FixedPoint* modules may be used with any of the IVP solvers (CVODE(S), IDA(S) and ARKODE) for complex-valued problems, the Anderson-acceleration option with SUNNonlinearSolver_FixedPoint cannot be used due to its reliance on `N_VDotProd()`. By this same logic, the Anderson acceleration feature within KINSOL will also not work with complex-valued vectors.

Finally, constraint-handling features of each package cannot be used for complex-valued data, due to the issue of ordering in the complex plane discussed above with `N_VCompare()`, `N_VConstrMask()`, `N_VMinQuotient()`, `N_VConstrMaskLocal()` and `N_VMinQuotientLocal()`.

We provide a simple example of a complex-valued example problem, including a custom complex-valued Fortran 2003 NVECTOR module, in the files `examples/arkode/F2003_custom/ark_analytic_complex_f2003.f90`, `examples/arkode/F2003_custom/fnvector_complex_mod.f90`, and `examples/arkode/F2003_custom/test_fnvector_complex_mod.f90`.

6.2 Description of the NVECTOR operations

6.2.1 Standard vector operations

The standard vector operations defined by the generic `N_Vector` module are defined as follows. For each of these operations, we give the name, usage of the function, and a description of its mathematical operations below.

N_Vector_ID **N_VGetVectorID**(*N_Vector* w)

> Returns the vector type identifier for the vector `w`. It is used to determine the vector implementation type (e.g. serial, parallel, ...) from the abstract `N_Vector` interface. Returned values are given in Table 6.1.
>
> Usage:
>
> ```
> id = N_VGetVectorID(w);
> ```

N_Vector **N_VClone**(*N_Vector* w)

> Creates a new `N_Vector` of the same type as an existing vector *w* and sets the *ops* field. It does not copy the vector, but rather allocates storage for the new vector.
>
> Usage:
>
> ```
> v = N_VClone(w);
> ```

N_Vector **N_VCloneEmpty**(*N_Vector* w)

> Creates a new `N_Vector` of the same type as an existing vector *w* and sets the *ops* field. It does not allocate storage for the new vector's data.
>
> Usage:
>
> ```
> v = N VCloneEmpty(w);
> ```

void **N_VDestroy**(*N_Vector* v)

> Destroys the `N_Vector` *v* and frees memory allocated for its internal data.
>
> Usage:
>
> ```
> N_VDestroy(v);
> ```

void **N_VSpace**(*N_Vector* v, *sunindextype* *lrw, *sunindextype* *liw)

> Returns storage requirements for the `N_Vector` *v*:
>
> - *lrw* contains the number of `realtype` words
> - *liw* contains the number of integer words.
>
> This function is advisory only, for use in determining a user's total space requirements; it could be a dummy function in a user-supplied NVECTOR module if that information is not of interest.
>
> Usage:
>
> ```
> N_VSpace(nvSpec, &lrw, &liw);
> ```

realtype ***N_VGetArrayPointer**(*N_Vector* v)

> Returns a pointer to a `realtype` array from the `N_Vector` *v*. Note that this assumes that the internal data in the `N_Vector` is a contiguous array of `realtype` and is accesible from the CPU.

This routine is only used in the solver-specific interfaces to the dense and banded (serial) linear solvers, and in the interfaces to the banded (serial) and band-block-diagonal (parallel) preconditioner modules provided with SUNDIALS.

Usage:

```
vdata = N_VGetArrayPointer(v);
```

realtype ***N_VGetDeviceArrayPointer**(*N_Vector* v)

Returns a device pointer to a `realtype` array from the `N_Vector` v. Note that this assumes that the internal data in `N_Vector` is a contiguous array of `realtype` and is accessible from the device (e.g., GPU).

This operation is *optional* except when using the GPU-enabled direct linear solvers.

Usage:

```
vdata = N_VGetArrayPointer(v);
```

void **N_VSetArrayPointer**(*realtype* *vdata, *N_Vector* v)

Replaces the data array pointer in an `N_Vector` with a given array of `realtype`. Note that this assumes that the internal data in the `N_Vector` is a contiguous array of `realtype`. This routine is only used in the interfaces to the dense (serial) linear solver, hence need not exist in a user-supplied NVECTOR module.

Usage:

```
N_VSetArrayPointer(vdata,v);
```

void ***N_VGetCommunicator**(*N_Vector* v)

Returns a pointer to the `MPI_Comm` object associated with the vector (if applicable). For MPI-unaware vector implementations, this should return NULL.

Usage:

```
commptr = N_VGetCommunicator(v);
```

sunindextype **N_VGetLength**(*N_Vector* v)

Returns the global length (number of "active" entries) in the NVECTOR *v*. This value should be cumulative across all processes if the vector is used in a parallel environment. If *v* contains additional storage, e.g., for parallel communication, those entries should not be included.

Usage:

```
global_length = N_VGetLength(v);
```

sunindextype **N_VGetLocalLength**(*N_Vector* v)

Returns the local length (number of "active" entries) in the NVECTOR *v*. This value should be the length of the array returned by *N_VGetArrayPointer()* or *N_VGetDeviceArrayPointer()*.

Usage:

```
local_length = N_VGetLocalLength(v);
```

void **N_VLinearSum**(*realtype* a, *N_Vector* x, *realtype* b, *N_Vector* y, *N_Vector* z)

Performs the operation $z = ax + by$, where a and b are `realtype` scalars and x and y are of type `N_Vector`:

$$z_i = ax_i + by_i, \quad i = 0, \ldots, n-1.$$

The output vector z can be the same as either of the input vectors (x or y).

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Usage:

```
N_VLinearSum(a, x, b, y, z);
```

void **N_VConst**(*realtype* c, *N_Vector* z)

Sets all components of the N_Vector z to realtype c:

$$z_i = c, \quad i = 0, \ldots, n - 1.$$

Usage:

```
N_VConst(c, z);
```

void **N_VProd**(*N_Vector* x, *N_Vector* y, *N_Vector* z)

Sets the N_Vector z to be the component-wise product of the N_Vector inputs x and y:

$$z_i = x_i y_i, \quad i = 0, \ldots, n - 1.$$

Usage:

```
N_VProd(x, y, z);
```

void **N_VDiv**(*N_Vector* x, *N_Vector* y, *N_Vector* z)

Sets the N_Vector z to be the component-wise ratio of the N_Vector inputs x and y:

$$z_i = \frac{x_i}{y_i}, \quad i = 0, \ldots, n - 1.$$

The y_i may not be tested for 0 values. It should only be called with a y that is guaranteed to have all nonzero components.

Usage:

```
N_VDiv(x, y, z);
```

void **N_VScale**(*realtype* c, *N_Vector* x, *N_Vector* z)

Scales the N_Vector x by the realtype scalar c and returns the result in z:

$$z_i = c x_i, \quad i = 0, \ldots, n - 1.$$

Usage:

```
N_VScale(c, x, z);
```

void **N_VAbs**(*N_Vector* x, *N_Vector* z)

Sets the components of the N_Vector z to be the absolute values of the components of the N_Vector x:

$$z_i = |x_i|, \quad i = 0, \ldots, n - 1.$$

Usage:

```
N_VAbs(x, z);
```

void **N_VInv**(*N_Vector* x, *N_Vector* z)

Sets the components of the N_Vector z to be the inverses of the components of the N_Vector x:

$$z_i = \frac{1}{x_i}, \quad i = 0, \ldots, n-1.$$

This routine may not check for division by 0. It should be called only with an x which is guaranteed to have all nonzero components.

Usage:

```
N_VInv(x, z);
```

void **N_VAddConst**(*N_Vector* x, *realtype* b, *N_Vector* z)

Adds the `realtype` scalar b to all components of x and returns the result in the N_Vector z:

$$z_i = x_i + b, \quad i = 0, \ldots, n-1.$$

Usage:

```
N_VAddConst(x, b, z);
```

realtype **N_VDotProd**(*N_Vector* x, *N_Vector* z)

Returns the value of the dot-product of the N_Vectors x and y:

$$d = \sum_{i=0}^{n-1} x_i y_i.$$

Usage:

```
d = N_VDotProd(x, y);
```

realtype **N_VMaxNorm**(*N_Vector* x)

Returns the value of the l_∞ norm of the N_Vector x:

$$m = \max_{0 \le i < n} |x_i|.$$

Usage:

```
m = N_VMaxNorm(x);
```

realtype **N_VWrmsNorm**(*N_Vector* x, *N_Vector* w)

Returns the weighted root-mean-square norm of the N_Vector x with (positive) `realtype` weight vector w:

$$m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i)^2 \right) / n}$$

Usage:

```
m = N_VWrmsNorm(x, w);
```

realtype **N_VWrmsNormMask**(*N_Vector* x, *N_Vector* w, *N_Vector* id)

Returns the weighted root mean square norm of the N_Vector x with `realtype` weight vector w built using only the elements of x corresponding to positive elements of the N_Vector *id*:

$$m = \sqrt{\left(\sum_{i=0}^{n-1} (x_i w_i H(id_i))^2 \right) / n},$$

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where $H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \leq 0 \end{cases}$.

Usage:

```
m = N_VWrmsNormMask(x, w, id);
```

realtype **N_VMin**(*N_Vector* x)

Returns the smallest element of the N_Vector x:

$$m = \min_{0 \leq i < n} x_i.$$

Usage:

```
m = N_VMin(x);
```

realtype **N_VWl2Norm**(*N_Vector* x, *N_Vector* w)

Returns the weighted Euclidean l_2 norm of the N_Vector x with realtype weight vector w:

$$m = \sqrt{\sum_{i=0}^{n-1} (x_i w_i)^2}.$$

Usage:

```
m = N_VWL2Norm(x, w);
```

realtype **N_VL1Norm**(*N_Vector* x)

Returns the l_1 norm of the N_Vector x:

$$m = \sum_{i=0}^{n-1} |x_i|.$$

Usage:

```
m = N_VL1Norm(x);
```

void **N_VCompare**(*realtype* c, *N_Vector* x, *N_Vector* z)

Compares the components of the N_Vector x to the realtype scalar c and returns an N_Vector z such that for all $0 \leq i < n$,

$$z_i = \begin{cases} 1.0 & \text{if } |x_i| \geq c, \\ 0.0 & \text{otherwise} \end{cases}.$$

Usage:

```
N_VCompare(c, x, z);
```

booleantype **N_VInvTest**(*N_Vector* x, *N_Vector* z)

Sets the components of the N_Vector z to be the inverses of the components of the N_Vector x, with prior testing for zero values:

$$z_i = \frac{1}{x_i}, \quad i = 0, \dots, n-1.$$

This routine returns a boolean assigned to SUNTRUE if all components of x are nonzero (successful inversion) and returns SUNFALSE otherwise.

Usage:

```
t = N_VInvTest(x, z);
```

booleantype **N_VConstrMask**(*N_Vector* c, *N_Vector* x, *N_Vector* m)

Performs the following constraint tests based on the values in c_i:

$$
\begin{array}{rcll}
x_i & > & 0 & \text{if} \quad c_i = 2, \\
x_i & \geq & 0 & \text{if} \quad c_i = 1, \\
x_i & < & 0 & \text{if} \quad c_i = -2, \\
x_i & \leq & 0 & \text{if} \quad c_i = -1.
\end{array}
$$

There is no constraint on x_i if $c_i = 0$. This routine returns a boolean assigned to SUNFALSE if any element failed the constraint test and assigned to SUNTRUE if all passed. It also sets a mask vector *m*, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.

Usage:

```
t = N_VConstrMask(c, x, m);
```

realtype **N_VMinQuotient**(*N_Vector* num, *N_Vector* denom)

This routine returns the minimum of the quotients obtained by termwise dividing the elements of *n* by the elements in *d*:

$$
\min_{0 \leq i < n} \frac{\text{num}_i}{\text{denom}_i}.
$$

A zero element in *denom* will be skipped. If no such quotients are found, then the large value BIG_REAL (defined in the header file sundials_types.h) is returned.

Usage:

```
minq = N_VMinQuotient(num, denom);
```

6.2.2 Fused operations

The following fused vector operations are *optional*. These operations are intended to increase data reuse, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. If a particular NVECTOR implementation defines one of the fused vector operations as NULL, the NVECTOR interface will call one of the above standard vector operations as necessary. As above, for each operation, we give the name, usage of the function, and a description of its mathematical operations below.

int **N_VLinearCombination**(int nv, *realtype* *c, *N_Vector* *X, *N_Vector* z)

This routine computes the linear combination of *nv* vectors with n elements:

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

where c is an array of nv scalars, x_j is a vector in the vector array *X*, and z is the output vector. If the output vector z is one of the vectors in *X*, then it *must* be the first vector in the vector array. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VLinearCombination(nv, c, X, z);
```

int **N_VScaleAddMulti**(int nv, *realtype* *c, *N_Vector* x, *N_Vector* *Y, *N_Vector* *Z)

This routine scales and adds one vector to *nv* vectors with n elements:

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

where c is an array of scalars, x is a vector, y_j is a vector in the vector array Y, and z_j is an output vector in the vector array Z. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VScaleAddMulti(nv, c, x, Y, Z);
```

int **N_VDotProdMulti**(int nv, *N_Vector* x, *N_Vector* *Y, *realtype* *d)

This routine computes the dot product of a vector with *nv* vectors having n elements:

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

where d is an array of scalars containing the computed dot products, x is a vector, and y_j is a vector the vector array Y. The operation returns 0 for success and a non-zero value otherwise.

Usage:

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

6.2.3 Vector array operations

The following vector array operations are also *optional*. As with the fused vector operations, these are intended to increase data reuse, reduce parallel communication on distributed memory systems, and lower the number of kernel launches on systems with accelerators. If a particular NVECTOR implementation defines one of the fused or vector array operations as NULL, the NVECTOR interface will call one of the above standard vector operations as necessary. As above, for each operation, we give the name, usage of the function, and a description of its mathematical operations below.

int **N_VLinearSumVectorArray**(int nv, *realtype* a, *N_Vector* X, *realtype* b, *N_Vector* *Y, *N_Vector* *Z)

This routine computes the linear sum of two vector arrays of *nv* vectors with n elements:

$$z_{j,i} = a x_{j,i} + b y_{j,i}, \quad i = 0, \ldots, n - 1 \quad j = 0, \ldots, nv - 1,$$

where a and b are scalars, x_j and y_j are vectors in the vector arrays X and Y respectively, and z_j is a vector in the output vector array Z. The operation returns 0 for success and a non-zero value otherwise.

Usage:

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

int **N_VScaleVectorArray**(int nv, *realtype* *c, *N_Vector* *X, *N_Vector* *Z)

This routine scales each element in a vector of n elements in a vector array of *nv* vectors by a potentially different constant:

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

where c is an array of scalars, x_j is a vector in the vector array X, and z_j is a vector in the output vector array Z. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VScaleVectorArray(nv, c, X, Z);
```

int **N_VConstVectorArray**(int nv, *realtype* c, *N_Vector* *Z)

This routine sets each element in a vector of n elements in a vector array of *nv* vectors to the same value:

$$z_{j,i} = c, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, nv-1,$$

where c is a scalar and z_j is a vector in the vector array Z. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VConstVectorArray(nv, c, Z);
```

int **N_VWrmsNormVectorArray**(int nv, *N_Vector* *X, *N_Vector* *W, *realtype* *m)

This routine computes the weighted root mean square norm of each vector in a vector array:

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

where x_j is a vector in the vector array X, w_j is a weight vector in the vector array W, and m is the output array of scalars containing the computed norms. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VWrmsNormVectorArray(nv, X, W, m);
```

int **N_VWrmsNormMaskVectorArray**(int nv, *N_Vector* *X, *N_Vector* *W, *N_Vector* id, *realtype* *m)

This routine computes the masked weighted root mean square norm of each vector in a vector array:

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

where $H(id_i) = 1$ if $id_i > 0$ and is zero otherwise, x_j is a vector in the vector array X, w_j is a weight vector in the vector array W, *id* is the mask vector, and m is the output array of scalars containing the computed norms. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VWrmsNormMaskVectorArray(nv, X, W, id, m);
```

int **N_VScaleAddMultiVectorArray**(int nv, int nsum, *realtype* *c, *N_Vector* *X, *N_Vector* **YY, *N_Vector* **ZZ)

This routine scales and adds a vector array of *nv* vectors to *nsum* other vector arrays:

$$z_{k,j,i} = c_k x_{j,i} + y_{k,j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, nv-1, \quad k = 0, \ldots, nsum-1$$

where c is an array of scalars, x_j is a vector in the vector array X, $y_{k,j}$ is a vector in the array of vector arrays YY, and $z_{k,j}$ is an output vector in the array of vector arrays ZZ. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VScaleAddMultiVectorArray(nv, nsum, c, x, YY, ZZ);
```

---

int **N_VLinearCombinationVectorArray**(int nv, int nsum, *realtype* *c, *N_Vector* **XX, *N_Vector* *Z)

This routine computes the linear combination of *nsum* vector arrays containing *nv* vectors:

$$z_{j,i} = \sum_{k=0}^{nsum-1} c_k x_{k,j,i}, \quad i = 0, \ldots, n-1 \quad j = 0, \ldots, nv-1,$$

where *c* is an array of scalars, $x_{k,j}$ is a vector in array of vector arrays *XX*, and $z_{j,i}$ is an output vector in the vector array *Z*. If the output vector array is one of the vector arrays in *XX*, it *must* be the first vector array in *XX*. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VLinearCombinationVectorArray(nv, nsum, c, XX, Z);
```

6.2.4 Local reduction operations

The following local reduction operations are also *optional*. As with the fused and vector array operations, these are intended to reduce parallel communication on distributed memory systems. If a particular NVECTOR implementation defines one of the local reduction operations as NULL, the NVECTOR interface will call one of the above standard vector operations as necessary. As above, for each operation, we give the name, usage of the function, and a description of its mathematical operations below.

realtype **N_VDotProdLocal**(*N_Vector* x, *N_Vector* y)

This routine computes the MPI task-local portion of the ordinary dot product of *x* and *y*:

$$d = \sum_{i=0}^{n_{local}-1} x_i y_i,$$

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

Usage:

```
d = N_VDotProdLocal(x, y);
```

realtype **N_VMaxNormLocal**(*N_Vector* x)

This routine computes the MPI task-local portion of the maximum norm of the NVECTOR *x*:

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

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

Usage:

```
m = N_VMaxNormLocal(x);
```

realtype **N_VMinLocal**(*N_Vector* x)

This routine computes the smallest element of the MPI task-local portion of the NVECTOR *x*:

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

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

Usage:

```
m = N_VMinLocal(x);
```

realtype **N_VL1NormLocal**(*N_Vector* x)

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

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

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

Usage:

```
n = N_VL1NormLocal(x);
```

realtype **N_VWSqrSumLocal**(*N_Vector* x, *N_Vector* w)

This routine computes the MPI task-local portion of the weighted squared sum of the NVECTOR *x* with weight vector *w*:

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

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

Usage:

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

realtype **N_VWSqrSumMaskLocal**(*N_Vector* x, *N_Vector* w, *N_Vector* id)

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

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

where

$$H(\alpha) = \begin{cases} 1 & \alpha > 0 \\ 0 & \alpha \le 0 \end{cases}$$

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

Usage:

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

booleantype **N_VInvTestLocal**(*N_Vector* x)

This routine sets the MPI task-local components of the NVECTOR *z* to be the inverses of the components of the NVECTOR *x*, with prior testing for zero values:

$$z_i = \frac{1}{x_i}, \; i = 0, \ldots, n_{local} - 1$$

where n_{local} corresponds to the number of components in the vector on this MPI task (or $n_{local} = n$ for MPI-unaware applications). This routine returns a boolean assigned to `SUNTRUE` if all task-local components of *x* are nonzero (successful inversion) and returns `SUNFALSE` otherwise.

Usage:

```
t = N_VInvTestLocal(x);
```

booleantype **N_VConstrMaskLocal**(*N_Vector* c, *N_Vector* x, *N_Vector* m)

Performs the following constraint tests based on the values in c_i:

$$
\begin{array}{rclcl}
x_i & > & 0 & \text{if} & c_i = 2, \\
x_i & \geq & 0 & \text{if} & c_i = 1, \\
x_i & < & 0 & \text{if} & c_i = -2, \\
x_i & \leq & 0 & \text{if} & c_i = -1.
\end{array}
$$

for all MPI task-local components of the vectors. This routine returns a boolean assigned to `SUNFALSE` if any task-local element failed the constraint test and assigned to `SUNTRUE` if all passed. It also sets a mask vector *m*, with elements equal to 1.0 where the constraint test failed, and 0.0 where the test passed. This routine is used only for constraint checking.

Usage:

```
t = N_VConstrMaskLocal(c, x, m);
```

realtype **N_VMinQuotientLocal**(*N_Vector* num, *N_Vector* denom)

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

Usage:

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

6.2.5 Single Buffer Reduction Operations

The following *optional* operations are used to combine separate reductions into a single MPI call by splitting the local computation and communication into separate functions. These operations are used in low-synchronization orthogonalization methods to reduce the number of MPI `Allreduce` calls. If a particular NVECTOR implementation does not define these operations additional communication will be required.

int **N_VDotProdMultiLocal**(int nv, *N_Vector* x, *N_Vector* *Y, *realtype* *d)

This routine computes the MPI task-local portion of the dot product of a vector *x* with *nv* vectors y_j:

$$
d_j = \sum_{i=0}^{n_{local}-1} x_i y_{j,i}, \quad j = 0, \ldots, nv - 1,
$$

where *d* is an array of scalars containing the computed dot products, *x* is a vector, y_j is a vector in the vector array *Y*, and n_{local} corresponds to the number of components in the vector on this MPI task. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VDotProdMultiLocal(nv, x, Y, d);
```

int **N_VDotProdMultiAllReduce**(int nv, *N_Vector* x, *realtype* *d)

This routine combines the MPI task-local portions of the dot product of a vector *x* with *nv* vectors:

```
retval = MPI_Allreduce(MPI_IN_PLACE, d, nv, MPI_SUNREALTYPE, MPI_SUM, comm)
```

where *d* is an array of *nv* scalars containing the local contributions to the dot product and *comm* is the MPI communicator associated with the vector *x*. The operation returns 0 for success and a non-zero value otherwise.

Usage:

```
retval = N_VDotProdMultiAllReduce(nv, x, d);
```

6.2.6 Exchange operations

The following vector exchange operations are also *optional* and are intended only for use when interfacing with the XBraid library for parallel-in-time integration. In that setting these operations are required but are otherwise unused by SUNDIALS packages and may be set to NULL. For each operation, we give the function signature, a description of the expected behavior, and an example of the function usage.

int **N_VBufSize**(*N_Vector* x, *sunindextype* *size)

This routine returns the buffer size need to exchange in the data in the vector *x* between computational nodes.

Usage:

```
flag = N_VBufSize(x, &buf_size)
```

int **N_VBufPack**(*N_Vector* x, void *buf)

This routine fills the exchange buffer *buf* with the vector data in *x*.

Usage:

```
flag = N_VBufPack(x, &buf)
```

int **N_VBufUnpack**(*N_Vector* x, void *buf)

This routine unpacks the data in the exchange buffer *buf* into the vector *x*.

Usage:

```
flag = N_VBufUnpack(x, buf)
```

6.3 NVECTOR functions used by CVODE

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

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

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

	CVODE	CVLS	CVDIAG	CVBANDPRE	CVBBDPRE
N_VGetVectorID()					
N_VGetLength()		4			
N_VClone()	x	x	x		
N_VCloneEmpty()		1			
N_VDestroy()	x	x	x		
N_VSpace()	x	2			
N_VGetArrayPointer()		1		x	x
N_VSetArrayPointer()		1			
N_VLinearSum()	x	x	x		
N_VConst()	x	x			
N_VProd()	x		x		
N_VDiv()	x		x		
N_VScale()	x	x	x	x	x
N_VAbs()	x				
N_VInv()	x		x		
N_VAddConst()	x		x		
N_VMaxNorm()	x				
N_VWrmsNorm()	x	x		x	x
N_VMin()	x				
N_VMinQuotient()	x				
N_VConstrMask()	x				
N_VCompare()	x		x		
N_VInvTest()			x		
N_VLinearCombination()	x				
N_VScaleAddMulti()	x				
N_VDotProdMulti()	3	3			
N_VScaleVectorArray()	x				

Special cases (numbers match markings in table):

1. These routines are only required if an internal difference-quotient routine for constructing *SUNMATRIX_DENSE* or *SUNMATRIX_BAND* Jacobian matrices is used.

2. This routine is optional, and is only used in estimating space requirements for CVODE modules for user feedback.

3. The optional function `N_VDotProdMulti` is only used in the SUNNONLINSOL_FIXEDPOINT module, or when Classical Gram-Schmidt is enabled with SPGMR or SPFGMR. The remaining operations from §6.2.2 – §6.2.3 not listed above are unused and a user-supplied NVECTOR module for CVODE could omit these operations.

4. This routine is only used when an iterative or matrix iterative SUNLINSOL module is supplied to CVODE.

Each SUNLINSOL object may require additional NVECTOR routines not listed in the table above. Please see the the relevant descriptions of these modules in §8 for additional detail on their NVECTOR requirements.

The vector functions listed in §6.2 that are *not* used by CVODE are: `N_VWL2Norm()`, *N_VDotProd()*, *N_VL1Norm()*, *N_VWrmsNormMask()*, and *N_VGetCommunicator()*. Therefore, a user-supplied NVECTOR module for CVODE could omit these functions (although some may be needed by SUNNONLINSOL or SUNLINSOL modules). The functions `N_MinQuotient()`, *N_VConstrMask()*, and *N_VCompare()* are only used when constraint checking is enabled and may be omitted if this feature is not used.

6.4 The NVECTOR_SERIAL Module

The serial implementation of the NVECTOR module provided with SUNDIALS, NVECTOR_SERIAL, defines the *content* field of an `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.

```c
struct _N_VectorContent_Serial {
    sunindextype length;
    booleantype own_data;
    realtype *data;
};
```

The header file to be included when using this module is `nvector_serial.h`. The installed module library to link to is `libsundials_nvecserial.lib` where `.lib` is typically `.so` for shared libraries and `.a` for static libraries.

6.4.1 NVECTOR_SERIAL accessor macros

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(v)

> This macro gives access to the contents of the serial vector `N_Vector` *v*.
>
> The assignment `v_cont = NV_CONTENT_S(v)` sets `v_cont` to be a pointer to the serial `N_Vector` *content* structure.
>
> Implementation:
>
> ```c
> #define NV_CONTENT_S(v) ( (N_VectorContent_Serial)(v->content) )
> ```

NV_OWN_DATA_S(v)

> Access the *own_data* component of the serial `N_Vector` *v*.
>
> Implementation:
>
> ```c
> #define NV_OWN_DATA_S(v) ( NV_CONTENT_S(v)->own_data )
> ```

NV_DATA_S(v)

> 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*.
>
> Similarly, the assignment `NV_DATA_S(v) = v_data` sets the component array of `v` to be `v_data` by storing the pointer `v_data`.
>
> Implementation:
>
> ```c
> #define NV_DATA_S(v) ( NV_CONTENT_S(v)->data )
> ```

NV_LENGTH_S(v)

> Access the *length* component of the serial `N_Vector` *v*.
>
> 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_LENGTH_S(v) ( NV_CONTENT_S(v)->length )
```

NV_Ith_S(v, i)

   This macro gives access to the individual components of the *data* array of an N_Vector, using standard 0-based C indexing.

   The assignment `r = NV_Ith_S(v,i)` sets `r` to be the value of the `i`-th component of `v`.

   The assignment `NV_Ith_S(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

   Here `i` ranges from 0 to $n - 1$ for a vector of length n.

   Implementation:

```
#define NV_Ith_S(v,i) ( NV_DATA_S(v)[i] )
```

6.4.2 NVECTOR_SERIAL functions

The NVECTOR_SERIAL module defines serial implementations of all vector operations listed in §6.2.1, §6.2.2, §6.2.3, and §6.2.4. Their names are obtained from those in those sections by appending the suffix `_Serial` (e.g. N_VDestroy_Serial). All the standard vector operations listed in §6.2.1 with the suffix `_Serial` appended are callable via the Fortran 2003 interface by prepending an F (e.g. FN_VDestroy_Serial).

The module NVECTOR_SERIAL provides the following additional user-callable routines:

N_Vector **N_VNew_Serial**(*sunindextype* vec_length, *SUNContext* sunctx)

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

N_Vector **N_VNewEmpty_Serial**(*sunindextype* vec_length, *SUNContext* sunctx)

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

N_Vector **N_VMake_Serial**(*sunindextype* vec_length, *realtype* *v_data, *SUNContext* sunctx)

   This function creates and allocates memory for a serial vector with user-provided data array, *v_data*.

   (This function does *not* allocate memory for v_data itself.)

void **N_VPrint_Serial**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Serial**(*N_Vector* v, *booleantype* tf)

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

Notes

- When looping over the components of an N_Vector v, it is more efficient to first obtain the component array via v_data = NV_DATA_S(v), or equivalently v_data = N_VGetArrayPointer(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* to SUNFALSE. The functions N_VDestroy_Serial() and N_VDestroyVectorArray_Serial() will not attempt to free the pointer data for any N_Vector with *own_data* set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.

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

6.4.3 NVECTOR_SERIAL Fortran Interface

The NVECTOR_SERIAL module provides a Fortran 2003 module for use from Fortran applications.

The `fnvector_serial_mod` Fortran module defines interfaces to all NVECTOR_SERIAL C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading F. For example, the function `N_VNew_Serial` is interfaced as `FN_VNew_Serial`.

The Fortran 2003 NVECTOR_SERIAL interface module can be accessed with the `use` statement, i.e. `use fnvector_serial_mod`, and linking to the library `libsundials_fnvectorserial_mod.lib` in addition to the C library. For details on where the library and module file `fnvector_serial_mod.mod` are installed see §11. We note that the module is accessible from the Fortran 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fnvectorserial_mod` library.

6.5 The NVECTOR_PARALLEL Module

The NVECTOR_PARALLEL implementation of the NVECTOR module provided with SUNDIALS is based on MPI. It defines the *content* field of an `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, an a boolean flag *own_data* indicating ownership of the data array *data*.

```
struct _N_VectorContent_Parallel {
    sunindextype local_length;
    sunindextype global_length;
    booleantype own_data;
    realtype *data;
    MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_parallel.h`. The installed module library to link to is `libsundials_nvecparallel.lib` where `.lib` is typically `.so` for shared libraries and `.a` for static libraries.

6.5.1 NVECTOR_PARALLEL accessor macros

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(v)

> This macro gives access to the contents of the parallel `N_Vector` *v*.
>
> The assignment `v_cont = NV_CONTENT_P(v)` sets `v_cont` to be a pointer to the `N_Vector` *content* structure of type `struct N_VectorContent_Parallel`.
>
> Implementation:
>
> ```
> #define NV_CONTENT_P(v) ( (N_VectorContent_Parallel)(v->content) )
> ```

NV_OWN_DATA_P(v)

> Access the *own_data* component of the parallel `N_Vector` *v*.
>
> Implementation:
>
> ```
> #define NV_OWN_DATA_P(v)    ( NV_CONTENT_P(v)->own_data )
> ```

NV_DATA_P(v)

> The assignment v_data = NV_DATA_P(v) sets v_data to be a pointer to the first component of the *local_data* for the N_Vector v.
>
> The assignment NV_DATA_P(v) = v_data sets the component array of v to be v_data by storing the pointer v_data into *data*.
>
> Implementation:

```
#define NV_DATA_P(v)        ( NV_CONTENT_P(v)->data )
```

NV_LOCLENGTH_P(v)

> The assignment v_llen = NV_LOCLENGTH_P(v) sets v_llen to be the length of the local part of v.
>
> The call NV_LOCLENGTH_P(v) = llen_v sets the *local_length* of v to be llen_v.
>
> Implementation:

```
#define NV_LOCLENGTH_P(v)  ( NV_CONTENT_P(v)->local_length )
```

NV_GLOBLENGTH_P(v)

> The assignment v_glen = NV_GLOBLENGTH_P(v) sets v_glen to be the *global_length* of the vector v.
>
> The call NV_GLOBLENGTH_P(v) = glen_v sets the *global_length* of v to be glen_v.
>
> Implementation:

```
#define NV_GLOBLENGTH_P(v) ( NV_CONTENT_P(v)->global_length )
```

NV_COMM_P(v)

> This macro provides access to the MPI communicator used by the parallel N_Vector *v*.
>
> Implementation:

```
#define NV_COMM_P(v) ( NV_CONTENT_P(v)->comm )
```

NV_Ith_P(v, i)

> This macro gives access to the individual components of the *local_data* array of an N_Vector.
>
> The assignment r = NV_Ith_P(v,i) sets r to be the value of the i-th component of the local part of v.
>
> The assignment NV_Ith_P(v,i) = r sets the value of the i-th component of the local part of v to be r.
>
> Here i ranges from 0 to $n - 1$, where n is the *local_length*.
>
> Implementation:

```
#define NV_Ith_P(v,i) ( NV_DATA_P(v)[i] )
```

6.5.2 NVECTOR_PARALLEL functions

The NVECTOR_PARALLEL module defines parallel implementations of all vector operations listed in §6.2. Their names are obtained from the generic names by appending the suffix _Parallel (e.g. N_VDestroy_Parallel). The module NVECTOR_PARALLEL provides the following additional user-callable routines:

N_Vector **N_VNew_Parallel**(MPI_Comm comm, *sunindextype* local_length, *sunindextype* global_length, *SUNContext* sunctx)

> This function creates and allocates memory for a parallel vector having global length *global_length*, having processor-local length *local_length*, and using the MPI communicator *comm*.

N_Vector **N_VNewEmpty_Parallel**(MPI_Comm comm, *sunindextype* local_length, *sunindextype* global_length, *SUNContext* sunctx)

>   This function creates a new parallel N_Vector with an empty (NULL) data array.

N_Vector **N_VMake_Parallel**(MPI_Comm comm, *sunindextype* local_length, *sunindextype* global_length, *realtype* *v_data, *SUNContext* sunctx)

>   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.)

sunindextype **N_VGetLocalLength_Parallel**(*N_Vector* v)

>   This function returns the local vector length.

void **N_VPrint_Parallel**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Parallel**(*N_Vector* v, *booleantype* tf)

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

Notes

- When looping over the components of an `N_Vector` v, it is more efficient to first obtain the local component array via `v_data = N_VGetArrayPointer(v)`, or equivalently `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* to SUNFALSE. The routines N_VDestroy_Parallel() and N_VDestroyVectorArray_‐ Parallel() will not attempt to free the pointer data for any `N_Vector` with *own_data* set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.

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

6.5.3 NVECTOR_PARALLEL Fortran Interface

The NVECTOR_PARALLEL module provides a Fortran 2003 module for use from Fortran applications.

The `fnvector_parallel_mod` Fortran module defines interfaces to all NVECTOR_PARALLEL C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading F. For example, the function N_VNew_Parallel is interfaced as FN_VNew_Parallel.

The Fortran 2003 NVECTOR_PARALLEL interface module can be accessed with the `use` statement, i.e. `use fn‐vector_parallel_mod`, and linking to the library `libsundials_fnvectorparallel_mod.lib` in addition to the C library. For details on where the library and module file `fnvector_parallel_mod.mod` are installed see §11. We note that the module is accessible from the Fortran 2003 SUNDIALS integrators *without* separately linking to the `libsundials_fnvectorparallel_mod` library.

6.6 The NVECTOR_OPENMP Module

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, the number of threads used is based on the supplied argument in the vector constructor.

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

The header file to be included when using this module is nvector_openmp.h. The installed module library to link to is libsundials_nvecopenmp.lib where .lib is typically .so for shared libraries and .a for static libraries. The Fortran module file to use when using the Fortran 2003 interface to this module is fnvector_openmp_mod.mod.

6.6.1 NVECTOR_OPENMP accessor macros

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(v)

> This macro gives access to the contents of the OpenMP vector N_Vector *v*.
>
> 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(v)

> Access the *own_data* component of the OpenMP N_Vector *v*.
>
> Implementation:
>
> ```
> #define NV_OWN_DATA_OMP(v) ( NV_CONTENT_OMP(v)->own_data )
> ```

NV_DATA_OMP(v)

> 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*.
>
> Similarly, the assignment NV_DATA_OMP(v) = v_data sets the component array of v to be v_data by storing the pointer v_data.
>
> Implementation:

```
#define NV_DATA_OMP(v) ( NV_CONTENT_OMP(v)->data )
```

NV_LENGTH_OMP(v)

Access the *length* component of the OpenMP `N_Vector` *v*.

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`.

Implementation:

```
#define NV_LENGTH_OMP(v) ( NV_CONTENT_OMP(v)->length )
```

NV_NUM_THREADS_OMP(v)

Access the *num_threads* component of the OpenMP `N_Vector` *v*.

The assignment `v_threads = NV_NUM_THREADS_OMP(v)` sets `v_threads` to be the *num_threads* of `v`. On the other hand, the call `NV_NUM_THREADS_OMP(v) = num_threads_v` sets the *num_threads* of `v` to be `num_-threads_v`.

Implementation:

```
#define NV_NUM_THREADS_OMP(v) ( NV_CONTENT_OMP(v)->num_threads )
```

NV_Ith_OMP(v, i)

This macro gives access to the individual components of the *data* array of an `N_Vector`, using standard 0-based C indexing.

The assignment `r = NV_Ith_OMP(v,i)` sets `r` to be the value of the `i`-th component of `v`.

The assignment `NV_Ith_OMP(v,i) = r` sets the value of the `i`-th component of `v` to be `r`.

Here `i` ranges from 0 to $n - 1$ for a vector of length n.

Implementation:

```
#define NV_Ith_OMP(v,i) ( NV_DATA_OMP(v)[i] )
```

6.6.2 NVECTOR_OPENMP functions

The NVECTOR_OPENMP module defines OpenMP implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4. Their names are obtained from those in those sections by appending the suffix _OpenMP (e.g. `N_-VDestroy_OpenMP`). All the standard vector operations listed in §6.2 with the suffix _OpenMP appended are callable via the Fortran 2003 interface by prepending an *F' (e.g. ``FN_VDestroy_OpenMP``).

The module NVECTOR_OPENMP provides the following additional user-callable routines:

N_Vector **N_VNew_OpenMP**(*sunindextype* vec_length, int num_threads, *SUNContext* sunctx)

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

N_Vector **N_VNewEmpty_OpenMP**(*sunindextype* vec_length, int num_threads, *SUNContext* sunctx)

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

N_Vector **N_VMake_OpenMP**(*sunindextype* vec_length, *realtype* *v_data, int num_threads, *SUNContext* sunctx)

This function creates and allocates memory for a OpenMP vector with user-provided data array, *v_data*.

(This function does *not* allocate memory for `v_data` itself.)

void **N_VPrint_OpenMP**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_OpenMP**(*N_Vector* v, *booleantype* tf)

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

Notes

- When looping over the components of an `N_Vector v`, it is more efficient to first obtain the component array via `v_data = N_VGetArrayPointer(v)`, or equivalently `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* to SUNFALSE. The functions `N_VDestroy_OpenMP()` and `N_VDestroyVectorArray_OpenMP()` will not attempt to free the pointer data for any `N_Vector` with *own_data* set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.

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

6.6.3 NVECTOR_OPENMP Fortran Interface

The NVECTOR_OPENMP module provides a Fortran 2003 module for use from Fortran applications.

The `fnvector_openmp_mod` Fortran module defines interfaces to all NVECTOR_OPENMP C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading F. For example, the function `N_VNew_OpenMP` is interfaced as `FN_VNew_OpenMP`.

The Fortran 2003 NVECTOR_OPENMP interface module can be accessed with the `use` statement, i.e. `use fnvector_openmp_mod`, and linking to the library `libsundials_fnvectoropenmp_mod.lib` in addition to the C library. For details on where the library and module file `fnvector_openmp_mod.mod` are installed see §11.

6.7 The NVECTOR_PTHREADS Module

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

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

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

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

6.7.1 NVECTOR_PTHREADS accessor macros

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(v)

> This macro gives access to the contents of the Pthreads vector N_Vector *v*.
>
> 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(v)

> Access the *own_data* component of the Pthreads N_Vector *v*.
>
> Implementation:
>
> ```
> #define NV_OWN_DATA_PT(v) ( NV_CONTENT_PT(v)->own_data )
> ```

NV_DATA_PT(v)

> 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.
>
> Similarly, the assignment NV_DATA_PT(v) = v_data sets the component array of v to be v_data by storing the pointer v_data.
>
> Implementation:
>
> ```
> #define NV_DATA_PT(v) ( NV_CONTENT_PT(v)->data )
> ```

NV_LENGTH_PT(v)

> Access the *length* component of the Pthreads N_Vector *v*.
>
> 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.
>
> Implementation:
>
> ```
> #define NV_LENGTH_PT(v) ( NV_CONTENT_PT(v)->length )
> ```

NV_NUM_THREADS_PT(v)

> Access the *num_threads* component of the Pthreads N_Vector *v*.
>
> The assignment v_threads = NV_NUM_THREADS_PT(v) sets v_threads to be the *num_threads* of v. On the other hand, the call NV_NUM_THREADS_PT(v) = num_threads_v sets the *num_threads* of v to be num_-threads_v.
>
> Implementation:
>
> ```
> #define NV_NUM_THREADS_PT(v) ( NV_CONTENT_PT(v)->num_threads )
> ```

NV_Ith_PT(v, i)

> This macro gives access to the individual components of the *data* array of an N_Vector, using standard 0-based C indexing.
>
> The assignment r = NV_Ith_PT(v,i) sets r to be the value of the i-th component of v.

The assignment `NV_Ith_PT(v,i) = r` sets the value of the i-th component of `v` to be `r`.

Here `i` ranges from 0 to $n-1$ for a vector of length n.

Implementation:

```
#define NV_Ith_PT(v,i) ( NV_DATA_PT(v)[i] )
```

6.7.2 NVECTOR_PTHREADS functions

The NVECTOR_PTHREADS module defines Pthreads implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4. Their names are obtained from those in those sections by appending the suffix `_Pthreads` (e.g. N_VDestroy_Pthreads). All the standard vector operations listed in §6.2 are callable via the Fortran 2003 interface by prepending an *F'* (e.g. ``FN_VDestroy_Pthreads``). The module NVECTOR_PTHREADS provides the following additional user-callable routines:

N_Vector **N_VNew_Pthreads**(*sunindextype* vec_length, int num_threads, *SUNContext* sunctx)

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

N_Vector **N_VNewEmpty_Pthreads**(*sunindextype* vec_length, int num_threads, *SUNContext* sunctx)

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

N_Vector **N_VMake_Pthreads**(*sunindextype* vec_length, *realtype* *v_data, int num_threads, *SUNContext* sunctx)

> This function creates and allocates memory for a Pthreads vector with user-provided data array, *v_data*.

> (This function does *not* allocate memory for `v_data` itself.)

void **N_VPrint_Pthreads**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Pthreads**(*N_Vector* v, *booleantype* tf)

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

Notes

- When looping over the components of an `N_Vector` v, it is more efficient to first obtain the component array via `v_data = N_VGetArrayPointer(v)`, or equivalently `v_data = NV_DATA_PT(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_Pthreads()*, *N_VMake_Pthreads()*, and N_VCloneVectorArrayEmpty_Pthreads() set the field *own_data* to SUNFALSE. The functions N_VDestroy_Pthreads() and N_VDestroyVectorArray_Pthreads() will not attempt to free the pointer data for any `N_Vector` with *own_data* set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the data pointer.

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

6.7.3 NVECTOR_PTHREADS Fortran Interface

The NVECTOR_PTHREADS module provides a Fortran 2003 module for use from Fortran applications.

The `fnvector_pthreads_mod` Fortran module defines interfaces to all NVECTOR_PTHREADS C functions using the intrinsic `iso_c_binding` module which provides a standardized mechanism for interoperating with C. As noted in the C function descriptions above, the interface functions are named after the corresponding C function, but with a leading `F`. For example, the function `N_VNew_Pthreads` is interfaced as `FN_VNew_Pthreads`.

The Fortran 2003 NVECTOR_PTHREADS interface module can be accessed with the `use` statement, i.e. `use fnvector_pthreads_mod`, and linking to the library `libsundials_fnvectorpthreads_mod.lib` in addition to the C library. For details on where the library and module file `fnvector_pthreads_mod.mod` are installed see §11.

6.8 The NVECTOR_PARHYP Module

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

```
struct _N_VectorContent_ParHyp {
  sunindextype local_length;
  sunindextype global_length;
  booleantype own_data;
  booleantype own_parvector;
  realtype *data;
  MPI_Comm comm;
  hypre_ParVector *x;
};
```

The header file to be included when using this module is `nvector_parhyp.h`. The installed module library to link to is `libsundials_nvecparhyp.lib` where `.lib` is typically `.so` for shared libraries and `.a` for static libraries.

Unlike native SUNDIALS vector types, NVECTOR_PARHYP does not provide macros to access its member variables. Note that NVECTOR_PARHYP requires SUNDIALS to be built with MPI support.

6.8.1 NVECTOR_PARHYP functions

The NVECTOR_PARHYP module defines implementations of all vector operations listed in §6.2 except for *N_VSetArrayPointer()* and *N_VGetArrayPointer()* because accessing raw vector data is handled by low-level HYPRE functions. As such, this vector is not available for use with SUNDIALS Fortran interfaces. When access to raw vector data is needed, one should extract the HYPRE vector first, and then use HYPRE methods to access the data. Usage examples of NVECTOR_PARHYP are provided in the `cvAdvDiff_non_ph.c` example programs for CVODE and the `ark_diurnal_kry_ph.c` example program for ARKODE.

The names of parhyp methods are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffix `_ParHyp` (e.g. `N_VDestroy_ParHyp`). The module NVECTOR_PARHYP provides the following additional user-callable routines:

N_Vector **N_VNewEmpty_ParHyp**(MPI_Comm comm, *sunindextype* local_length, *sunindextype* global_length, *SUNContext* sunctx)

> This function creates a new parhyp `N_Vector` with the pointer to the HYPRE vector set to `NULL`.

N_Vector **N_VMake_ParHyp**(hypre_ParVector *x, *SUNContext* sunctx)

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

hypre_ParVector ***N_VGetVector_ParHyp**(*N_Vector* v)

> This function returns a pointer to the underlying HYPRE vector.

void **N_VPrint_ParHyp**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_ParHyp**(*N_Vector* v, *booleantype* tf)

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

Notes

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

- *N_VNewEmpty_ParHyp()*, *N_VMake_ParHyp()*, and N_VCloneVectorArrayEmpty_ParHyp() set the field *own_parvector* to SUNFALSE. The functions N_VDestroy_ParHyp() and N_VDestroyVectorArray_-ParHyp() will not attempt to delete an underlying HYPRE vector for any `N_Vector` with *own_parvector* set to SUNFALSE. In such a case, it is the user's responsibility to delete the underlying vector.

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

6.9 The NVECTOR_PETSC Module

The NVECTOR_PETSC module is an NVECTOR wrapper around the PETSc vector. It defines the *content* field of a `N_Vector` to be a structure containing the global and local lengths of the vector, a pointer to the PETSc vector, an MPI communicator, and a boolean flag *own_data* indicating ownership of the wrapped PETSc vector.

```
struct _N_VectorContent_Petsc {
    sunindextype local_length;
    sunindextype global_length;
    booleantype own_data;
    Vec *pvec;
    MPI_Comm comm;
};
```

The header file to be included when using this module is `nvector_petsc.h`. The installed module library to link to is `libsundials_nvecpetsc.lib` where `.lib` is typically `.so` for shared libraries and `.a` for static libraries.

Unlike native SUNDIALS vector types, NVECTOR_PETSC does not provide macros to access its member variables. Note that NVECTOR_PETSC requires SUNDIALS to be built with MPI support.

6.9.1 NVECTOR_PETSC functions

The NVECTOR_PETSC module defines implementations of all vector operations listed in §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 is provided in example programs for IDA.

The names of vector operations are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffice `_Petsc` (e.g. N_VDestroy_Petsc). The module NVECTOR_PETSC provides the following additional user-callable routines:

N_Vector **N_VNewEmpty_Petsc**(MPI_Comm comm, *sunindextype* local_length, *sunindextype* global_length, *SUNContext* sunctx)

    This function creates a new PETSC `N_Vector` with the pointer to the wrapped PETSc vector set to `NULL`. It is used by the `N_VMake_Petsc` and `N_VClone_Petsc` implementations. It should be used only with great caution.

N_Vector **N_VMake_Petsc**(Vec *pvec, *SUNContext* sunctx)

    This function creates and allocates memory for an NVECTOR_PETSC wrapper with a user-provided PETSc vector. It does *not* allocate memory for the vector `pvec` itself.

Vec ***N_VGetVector_Petsc**(*N_Vector* v)

    This function returns a pointer to the underlying PETSc vector.

void **N_VPrint_Petsc**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Petsc**(*N_Vector* v, *booleantype* tf)

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

Notes

- When there is a need to access components of an `N_Vector_Petsc` v, it is recommeded to extract the PETSc vector via `x_vec = N_VGetVector_Petsc(v);` and then access components using appropriate PETSc functions.

- The functions *N_VNewEmpty_Petsc()*, *N_VMake_Petsc()*, and N_VCloneVectorArrayEmpty_Petsc() set the field *own_data* to SUNFALSE. The routines N_VDestroy_Petsc() and N_VDestroyVectorArray_Petsc() will not attempt to free the pointer `pvec` for any `N_Vector` with *own_data* set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the `pvec` pointer.

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

6.10 The NVECTOR_CUDA Module

The NVECTOR_CUDA module is an NVECTOR implementation in the CUDA language. The module allows for SUNDIALS vector kernels to run on NVIDIA GPU devices. It is intended for users who are already familiar with CUDA and GPU programming. Building this vector module requires a CUDA compiler and, by extension, a C++ compiler. The vector content layout is as follows:

```
struct _N_VectorContent_Cuda
{
    sunindextype       length;
    booleantype        own_helper;
    SUNMemory          host_data;
    SUNMemory          device_data;
    SUNCudaExecPolicy* stream_exec_policy;
```

```
    SUNCudaExecPolicy* reduce_exec_policy;
    SUNMemoryHelper    mem_helper;
    void*              priv; /* 'private' data */
};

typedef struct _N_VectorContent_Cuda *N_VectorContent_Cuda;
```

The content members are the vector length (size), boolean flags that indicate if the vector owns the execution policies and memory helper objects (i.e., it is in change of freeing the objects), *SUNMemory* objects for the vector data on the host and device, pointers to execution policies that control how streaming and reduction kernels are launched, a *SUNMemoryHelper* for performing memory operations, and a private data structure which holds additonal members that should not be accessed directly.

When instantiated with *N_VNew_Cuda()*, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the *N_VMake_Cuda()* constructor. To use CUDA managed memory, the constructors *N_VNewManaged_Cuda()* and *N_VMakeManaged_Cuda()* are provided. Additionally, a user-defined SUNMemoryHelper for allocating/freeing data can be provided with the constructor *N_VNewWith-MemHelp_Cuda()*. Details on each of these constructors are provided below.

To use the NVECTOR_CUDA module, include `nvector_cuda.h` and link to the library `libsundials_nveccuda.lib`. The extension, `.lib`, is typically `.so` for shared libraries and `.a` for static libraries.

6.10.1 NVECTOR_CUDA functions

Unlike other native SUNDIALS vector types, the NVECTOR_CUDA module does not provide macros to access its member variables. Instead, user should use the accessor functions:

realtype ***N_VGetHostArrayPointer_Cuda**(*N_Vector* v)

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

realtype ***N_VGetDeviceArrayPointer_Cuda**(*N_Vector* v)

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

booleantype **N_VIsManagedMemory_Cuda**(*N_Vector* v)

> This function returns a boolean flag indiciating if the vector data array is in managed memory or not.

The NVECTOR_CUDA module defines implementations of all standard vector operations defined in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VSetArrayPointer()*, and, if using unmanaged memory, *N_VGetArrayPointer()*. As such, this vector can only be used with SUNDIALS direct solvers and preconditioners when using managed memory. The NVECTOR_CUDA module provides separate functions to access data on the host and on the device for the unmanaged memory use case. It also provides methods for copying from the host to the device and vice versa. Usage examples of NVECTOR_CUDA are provided in example programs for CVODE [40].

The names of vector operations are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffix _Cuda (e.g. N_VDestroy_Cuda). The module NVECTOR_CUDA provides the following additional user-callable routines:

N_Vector **N_VNew_Cuda**(*sunindextype* length, *SUNContext* sunctx)

> This function creates and allocates memory for a CUDA N_Vector. The vector data array is allocated on both the host and device.

N_Vector **N_VNewManaged_Cuda**(*sunindextype* vec_length, *SUNContext* sunctx)

> This function creates and allocates memory for a CUDA N_Vector. The vector data array is allocated in managed memory.

N_Vector **N_VNewWithMemHelp_Cuda**(*sunindextype* length, *booleantype* use_managed_mem, *SUNMemoryHelper* helper, *SUNContext* sunctx)

This function creates a new CUDA N_Vector with a user-supplied SUNMemoryHelper for allocating/freeing memory.

N_Vector **N_VNewEmpty_Cuda**(*sunindextype* vec_length, *SUNContext* sunctx)

This function creates a new CUDA N_Vector where the members of the content structure have not been allocated. This utility function is used by the other constructors to create a new vector.

N_Vector **N_VMake_Cuda**(*sunindextype* vec_length, *realtype* *h_vdata, *realtype* *d_vdata, *SUNContext* sunctx)

This function creates a CUDA N_Vector with user-supplied vector data arrays for the host and the device.

N_Vector **N_VMakeManaged_Cuda**(*sunindextype* vec_length, *realtype* *vdata, *SUNContext* sunctx)

This function creates a CUDA N_Vector with a user-supplied managed memory data array.

N_Vector **N_VMakeWithManagedAllocator_Cuda**(*sunindextype* length, void *(*allocfn)(size_t size), void (*freefn)(void *ptr))

This function creates a CUDA N_Vector with a user-supplied memory allocator. It requires the user to provide a corresponding free function as well. The memory allocated by the allocator function must behave like CUDA managed memory.

The module NVECTOR_CUDA also provides the following user-callable routines:

void **N_VSetKernelExecPolicy_Cuda**(*N_Vector* v, SUNCudaExecPolicy *stream_exec_policy, SUNCudaExecPolicy *reduce_exec_policy)

This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction CUDA kernels. By default the vector is setup to use the *SUNCudaThreadDirectExecPolicy()* and *SUNCudaBlockReduceAtomicExecPolicy()*. Any custom execution policy for reductions must ensure that the grid dimensions (number of thread blocks) is a multiple of the CUDA warp size (32). See §6.10.2 below for more information about the *SUNCudaExecPolicy* class. Providing NULL for an argument will result in the default policy being restored.

The input execution policies are cloned and, as such, may be freed after being attached to the desired vectors. A NULL input policy will reset the execution policy to the default setting.

Note: Note: All vectors used in a single instance of a SUNDIALS package must use the same execution policy. It is **strongly recommended** that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors

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realtype ***N_VCopyToDevice_Cuda**(*N_Vector* v)

This function copies host vector data to the device.

realtype ***N_VCopyFromDevice_Cuda**(*N_Vector* v)

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

void **N_VPrint_Cuda**(*N_Vector* v)

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

void **N_VPrintFile_Cuda**(*N_Vector* v, FILE *outfile)

This function prints the content of a CUDA vector to outfile.

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

---

the same enable/disable options as the vector they are cloned from while vectors created with *N_VNew_Cuda()* will have the default settings for the NVECTOR_CUDA module.

int **N_VEnableFusedOps_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Cuda**(*N_Vector* v, *booleantype* tf)

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

Notes

- When there is a need to access components of an N_Vector_Cuda, v, it is recommeded to use functions *N_-VGetDeviceArrayPointer_Cuda()* or *N_VGetHostArrayPointer_Cuda()*. However, when using managed memory, the function *N_VGetArrayPointer()* may also be used.

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

6.10.2 The `SUNCudaExecPolicy` Class

In order to provide maximum flexibility to users, the CUDA kernel execution parameters used by kernels within SUN-DIALS are defined by objects of the `sundials::cuda::ExecPolicy` abstract class type (this class can be accessed in the global namespace as `SUNCudaExecPolicy`). Thus, users may provide custom execution policies that fit the needs of their problem. The SUNCudaExecPolicy class is defined as

typedef sundials::cuda::ExecPolicy **SUNCudaExecPolicy**

where the `sundials::cuda::ExecPolicy` class is defined in the header file `sundials_cuda_policies.hpp`, as follows:

```
class ExecPolicy
{
public:
   ExecPolicy(cudaStream_t stream = 0) : stream_(stream) { }
   virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
   virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
   virtual const cudaStream_t* stream() const { return (&stream_); }
   virtual ExecPolicy* clone() const = 0;
   ExecPolicy* clone_new_stream(cudaStream_t stream) const {
      ExecPolicy* ex = clone();
      ex->stream_ = stream;
      return ex;
   }
   virtual bool atomic() const { return false; }
   virtual ~ExecPolicy() {}
protected:
   cudaStream_t stream_;
};
```

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided `sundials::cuda::ThreadDirectExecPolicy` (aka in the global namespace as `SUNCudaThreadDirectExecPolicy`) class is a good example of a what a custom execution policy may look like:

```
class ThreadDirectExecPolicy : public ExecPolicy
{
public:
   ThreadDirectExecPolicy(const size_t blockDim, cudaStream_t stream = 0)
      : blockDim_(blockDim), ExecPolicy(stream)
   {}

   ThreadDirectExecPolicy(const ThreadDirectExecPolicy& ex)
      : blockDim_(ex.blockDim_), ExecPolicy(ex.stream_)
   {}

   virtual size_t gridSize(size_t numWorkUnits = 0, size_t /*blockDim*/ = 0) const
   {
      /* ceil(n/m) = floor((n + m - 1) / m) */
      return (numWorkUnits + blockSize() - 1) / blockSize();
   }

   virtual size_t blockSize(size_t /*numWorkUnits*/ = 0, size_t /*gridDim*/ = 0) const
```

```
   {
      return blockDim_;
   }

   virtual ExecPolicy* clone() const
   {
      return static_cast<ExecPolicy*>(new ThreadDirectExecPolicy(*this));
   }

private:
   const size_t blockDim_;
};
```

In total, SUNDIALS provides 3 execution policies:

SUNCudaThreadDirectExecPolicy(const size_t blockDim, const cudaStream_t stream = 0)

> Maps each CUDA thread to a work unit. The number of threads per block (blockDim) can be set to anything. The grid size will be calculated so that there are enough threads for one thread per element. If a CUDA stream is provided, it will be used to execute the kernel.

SUNCudaGridStrideExecPolicy(const size_t blockDim, const size_t gridDim, const cudaStream_t stream = 0)

> Is for kernels that use grid stride loops. The number of threads per block (blockDim) can be set to anything. The number of blocks (gridDim) can be set to anything. If a CUDA stream is provided, it will be used to execute the kernel.

SUNCudaBlockReduceExecPolicy(const size_t blockDim, const cudaStream_t stream = 0)

> Is for kernels performing a reduction across indvidual thread blocks. The number of threads per block (blockDim) can be set to any valid multiple of the CUDA warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a CUDA stream is provided, it will be used to execute the kernel.

SUNCudaBlockReduceAtomicExecPolicy(const size_t blockDim, const cudaStream_t stream = 0)

> Is for kernels performing a reduction across indvidual thread blocks using atomic operations. The number of threads per block (blockDim) can be set to any valid multiple of the CUDA warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a CUDA stream is provided, it will be used to execute the kernel.

For example, a policy that uses 128 threads per block and a user provided stream can be created like so:

```
cudaStream_t stream;
cudaStreamCreate(&stream);
SUNCudaThreadDirectExecPolicy thread_direct(128, stream);
```

These default policy objects can be reused for multiple SUNDIALS data structures (e.g. a *SUNMatrix* and an *N_-Vector*) since they do not hold any modifiable state information.

6.11 The NVECTOR_HIP Module

The NVECTOR_HIP module is an NVECTOR implementation using the AMD ROCm HIP library [1]. The module allows for SUNDIALS vector kernels to run on AMD or NVIDIA GPU devices. It is intended for users who are already familiar with HIP and GPU programming. Building this vector module requires the HIP-clang compiler. The vector content layout is as follows:

```
struct _N_VectorContent_Hip
{
    sunindextype       length;
    booleantype        own_helper;
    SUNMemory          host_data;
    SUNMemory          device_data;
    SUNHipExecPolicy*  stream_exec_policy;
    SUNHipExecPolicy*  reduce_exec_policy;
    SUNMemoryHelper    mem_helper;
    void*              priv; /* 'private' data */
};

typedef struct _N_VectorContent_Hip *N_VectorContent_Hip;
```

The content members are the vector length (size), a boolean flag that signals if the vector owns the data (i.e. it is in charge of freeing the data), pointers to vector data on the host and the device, pointers to *SUNHipExecPolicy* implementations that control how the HIP kernels are launched for streaming and reduction vector kernels, and a private data structure which holds additonal members that should not be accessed directly.

When instantiated with *N_VNew_Hip()*, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the *N_VMake_Hip()* constructor. To use managed memory, the constructors *N_VNewManaged_Hip()* and *N_VMakeManaged_Hip()* are provided. Additionally, a user-defined SUNMemoryHelper for allocating/freeing data can be provided with the constructor *N_VNewWithMemHelp_-Hip()*. Details on each of these constructors are provided below.

To use the NVECTOR_HIP module, include nvector_hip.h and link to the library libsundials_nvechip.lib. The extension, .lib, is typically .so for shared libraries and .a for static libraries.

6.11.1 NVECTOR_HIP functions

Unlike other native SUNDIALS vector types, the NVECTOR_HIP module does not provide macros to access its member variables. Instead, user should use the accessor functions:

realtype ***N_VGetHostArrayPointer_Hip**(*N_Vector* v)

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

realtype ***N_VGetDeviceArrayPointer_Hip**(*N_Vector* v)

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

booleantype **N_VIsManagedMemory_Hip**(*N_Vector* v)

> This function returns a boolean flag indiciating if the vector data array is in managed memory or not.

The NVECTOR_HIP module defines implementations of all standard vector operations defined in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VSetArrayPointer()*. The names of vector operations are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffix _Hip (e.g. N_VDestroy_Hip()). The module NVECTOR_HIP provides the following additional user-callable routines:

N_Vector **N_VNew_Hip**(*sunindextype* length, *SUNContext* sunctx)

> This function creates and allocates memory for a HIP N_Vector. The vector data array is allocated on both the host and device.

N_Vector **N_VNewManaged_Hip**(*sunindextype* vec_length, *SUNContext* sunctx)

> This function creates and allocates memory for a HIP N_Vector. The vector data array is allocated in managed memory.

N_Vector **N_VNewWithMemHelp_Hip**(*sunindextype* length, *booleantype* use_managed_mem, *SUNMemoryHelper* helper, *SUNContext* sunctx)

> This function creates a new HIP N_Vector with a user-supplied SUNMemoryHelper for allocating/freeing memory.

N_Vector **N_VNewEmpty_Hip**(*sunindextype* vec_length, *SUNContext* sunctx)

> This function creates a new HIP N_Vector where the members of the content structure have not been allocated. This utility function is used by the other constructors to create a new vector.

N_Vector **N_VMake_Hip**(*sunindextype* vec_length, *realtype* *h_vdata, *realtype* *d_vdata, *SUNContext* sunctx)

> This function creates a HIP N_Vector with user-supplied vector data arrays for the host and the device.

N_Vector **N_VMakeManaged_Hip**(*sunindextype* vec_length, *realtype* *vdata, *SUNContext* sunctx)

> This function creates a HIP N_Vector with a user-supplied managed memory data array.

The module NVECTOR_HIP also provides the following user-callable routines:

void **N_VSetKernelExecPolicy_Hip**(*N_Vector* v, SUNHipExecPolicy *stream_exec_policy, SUNHipExecPolicy *reduce_exec_policy)

> This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction HIP kernels. By default the vector is setup to use the *SUNHipThreadDirectExecPolicy()* and *SUNHipBlockReduceExecPolicy()*. Any custom execution policy for reductions must ensure that the grid dimensions (number of thread blocks) is a multiple of the HIP warp size (32 for NVIDIA GPUs, 64 for AMD GPUs). See §6.11.2 below for more information about the *SUNHipExecPolicy* class. Providing NULL for an argument will result in the default policy being restored.

> The input execution policies are cloned and, as such, may be freed after being attached to the desired vectors. A NULL input policy will reset the execution policy to the default setting.

> **Note:** Note: All vectors used in a single instance of a SUNDIALS package must use the same execution policy. It is **strongly recommended** that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors*

---

realtype ***N_VCopyToDevice_Hip**(*N_Vector* v)

> This function copies host vector data to the device.

realtype ***N_VCopyFromDevice_Hip**(*N_Vector* v)

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

void **N_VPrint_Hip**(*N_Vector* v)

> This function prints the content of a HIP vector to stdout.

void **N_VPrintFile_Hip**(*N_Vector* v, FILE *outfile)

> This function prints the content of a HIP vector to outfile.

By default all fused and vector array operations are disabled in the NVECTOR_HIP module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with *N_VNew_Hip()*, enable/disable the

desired operations for that vector with the functions below, and create any additional vectors from that vector using *N_-VClone()*. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created with *N_VNew_Hip()* will have the default settings for the NVECTOR_HIP module.

int **N_VEnableFusedOps_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Hip**(*N_Vector* v, *booleantype* tf)

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

Notes

- When there is a need to access components of an `N_Vector_Hip`, v, it is recommeded to use functions *N_-VGetDeviceArrayPointer_Hip()* or *N_VGetHostArrayPointer_Hip()*. However, when using managed memory, the function *N_VGetArrayPointer()* may also be used.

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

6.11.2 The `SUNHipExecPolicy` Class

In order to provide maximum flexibility to users, the HIP kernel execution parameters used by kernels within SUNDIALS are defined by objects of the `sundials::hip::ExecPolicy` abstract class type (this class can be accessed in the global namespace as `SUNHipExecPolicy`). Thus, users may provide custom execution policies that fit the needs of their problem. The `SUNHipExecPolicy` class is defined as

typedef sundials::hip::ExecPolicy **SUNHipExecPolicy**

where the `sundials::hip::ExecPolicy` class is defined in the header file `sundials_hip_policies.hpp`, as follows:

```cpp
class ExecPolicy
{
public:
   ExecPolicy(hipStream_t stream = 0) : stream_(stream) { }
   virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
   virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
   virtual const hipStream_t* stream() const { return (&stream_); }
   virtual ExecPolicy* clone() const = 0;
   ExecPolicy* clone_new_stream(hipStream_t stream) const {
      ExecPolicy* ex = clone();
      ex->stream_ = stream;
      return ex;
   }
   virtual bool atomic() const { return false; }
   virtual ~ExecPolicy() {}
protected:
   hipStream_t stream_;
};
```

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided `sundials::hip::ThreadDirectExecPolicy` (aka in the global namespace as `SUNHipThreadDirectExecPolicy`) class is a good example of a what a custom execution policy may look like:

```cpp
class ThreadDirectExecPolicy : public ExecPolicy
{
public:
   ThreadDirectExecPolicy(const size_t blockDim, hipStream_t stream = 0)
      : blockDim_(blockDim), ExecPolicy(stream)
   {}

   ThreadDirectExecPolicy(const ThreadDirectExecPolicy& ex)
      : blockDim_(ex.blockDim_), ExecPolicy(ex.stream_)
   {}

   virtual size_t gridSize(size_t numWorkUnits = 0, size_t /*blockDim*/ = 0) const
   {
```

(continues on next page)

```cpp
        /* ceil(n/m) = floor((n + m - 1) / m) */
        return (numWorkUnits + blockSize() - 1) / blockSize();
    }

    virtual size_t blockSize(size_t /*numWorkUnits*/ = 0, size_t /*gridDim*/ = 0) const
    {
        return blockDim_;
    }

    virtual ExecPolicy* clone() const
    {
        return static_cast<ExecPolicy*>(new ThreadDirectExecPolicy(*this));
    }

private:
    const size_t blockDim_;
};
```

In total, SUNDIALS provides 4 execution policies:

SUNHipThreadDirectExecPolicy(const size_t blockDim, const hipStream_t stream = 0)

> Maps each HIP thread to a work unit. The number of threads per block (blockDim) can be set to anything. The grid size will be calculated so that there are enough threads for one thread per element. If a HIP stream is provided, it will be used to execute the kernel.

SUNHipGridStrideExecPolicy(const size_t blockDim, const size_t gridDim, const hipStream_t stream = 0)

> Is for kernels that use grid stride loops. The number of threads per block (blockDim) can be set to anything. The number of blocks (gridDim) can be set to anything. If a HIP stream is provided, it will be used to execute the kernel.

SUNHipBlockReduceExecPolicy(const size_t blockDim, const hipStream_t stream = 0)

> Is for kernels performing a reduction across indvidual thread blocks. The number of threads per block (blockDim) can be set to any valid multiple of the HIP warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a HIP stream is provided, it will be used to execute the kernel.

SUNHipBlockReduceAtomicExecPolicy(const size_t blockDim, const hipStream_t stream = 0)

> Is for kernels performing a reduction across indvidual thread blocks using atomic operations. The number of threads per block (blockDim) can be set to any valid multiple of the HIP warp size. The grid size (gridDim) can be set to any value greater than 0. If it is set to 0, then the grid size will be chosen so that there is enough threads for one thread per work unit. If a HIP stream is provided, it will be used to execute the kernel.

For example, a policy that uses 128 threads per block and a user provided stream can be created like so:

```cpp
hipStream_t stream;
hipStreamCreate(&stream);
SUNHipThreadDirectExecPolicy thread_direct(128, stream);
```

These default policy objects can be reused for multiple SUNDIALS data structures (e.g. a *SUNMatrix* and an *N_-Vector*) since they do not hold any modifiable state information.

6.12 The NVECTOR_SYCL Module

The NVECTOR_SYCL module is an experimental NVECTOR implementation using the SYCL abstraction layer. At present the only supported SYCL compiler is the DPC++ (Intel oneAPI) compiler. This module allows for SUNDIALS vector kernels to run on Intel GPU devices. The module is intended for users who are already familiar with SYCL and GPU programming.

The vector content layout is as follows:

```
struct _N_VectorContent_Sycl
{
   sunindextype      length;
   booleantype       own_helper;
   SUNMemory         host_data;
   SUNMemory         device_data;
   SUNSyclExecPolicy* stream_exec_policy;
   SUNSyclExecPolicy* reduce_exec_policy;
   SUNMemoryHelper   mem_helper;
   sycl::queue*      queue;
   void*             priv; /* 'private' data */
};

typedef struct _N_VectorContent_Sycl *N_VectorContent_Sycl;
```

The content members are the vector length (size), boolean flags that indicate if the vector owns the execution policies and memory helper objects (i.e., it is in charge of freeing the objects), *SUNMemory* objects for the vector data on the host and device, pointers to execution policies that control how streaming and reduction kernels are launched, a *SUNMemoryHelper* for performing memory operations, the SYCL queue, and a private data structure which holds additional members that should not be accessed directly.

When instantiated with *N_VNew_Sycl()*, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the *N_VMake_Sycl()* constructor. To use managed (shared) memory, the constructors *N_VNewManaged_Sycl()* and *N_VMakeManaged_Sycl()* are provided. Additionally, a user-defined SUNMemoryHelper for allocating/freeing data can be provided with the constructor *N_VNewWith-MemHelp_Sycl()*. Details on each of these constructors are provided below.

The header file to include when using this is nvector_sycl.h. The installed module library to link to is libsundials_nvecsycl.lib. The extension .lib is typically .so for shared libraries .a for static libraries.

6.12.1 NVECTOR_SYCL functions

The NVECTOR_SYCL module implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VDotProdMulti()*, *N_VWrmsNormVectorArray()*, *N_VWrmsNormMaskVectorArray()* as support for arrays of reduction vectors is not yet supported. These functions will be added to the NVECTOR_SYCL implementation in the future. The names of vector operations are obtained from those in the aforementioned sections by appending the suffix _Sycl (e.g., N_VDestroy_Sycl).

Additionally, the NVECTOR_SYCL module provides the following user-callable constructors for creating a new NVECTOR_SYCL:

N_Vector **N_VNew_Sycl**(sunindextype vec_length, sycl::queue *Q, SUNContext sunctx)

> This function creates and allocates memory for an NVECTOR_SYCL. Vector data arrays are allocated on both the host and the device associated with the input queue. All operation are launched in the provided queue.

N_Vector **N_VNewManaged_Sycl**(sunindextype vec_length, sycl::queue *Q, SUNContext sunctx)

> This function creates and allocates memory for a NVECTOR_SYCL. The vector data array is allocated in managed (shared) memory using the input queue. All operation are launched in the provided queue.

N_Vector **N_VMake_Sycl**(sunindextype length, realtype *h_vdata, realtype *d_vdata, sycl::queue *Q, SUNContext sunctx)

> This function creates an NVECTOR_SYCL with user-supplied host and device data arrays. This function does not allocate memory for data itself. All operation are launched in the provided queue.

N_Vector **N_VMakeManaged_Sycl**(sunindextype length, realtype *vdata, sycl::queue *Q, SUNContext sunctx)

> This function creates an NVECTOR_SYCL with a user-supplied managed (shared) data array. This function does not allocate memory for data itself. All operation are launched in the provided queue.

N_Vector **N_VNewWithMemHelp_Sycl**(sunindextype length, booleantype use_managed_mem, SUNMemoryHelper helper, sycl::queue *Q, SUNContext sunctx)

> This function creates an NVECTOR_SYCL with a user-supplied SUNMemoryHelper for allocating/freeing memory. All operation are launched in the provided queue.

N_Vector **N_VNewEmpty_Sycl**()

> This function creates a new N_Vector where the members of the content structure have not been allocated. This utility function is used by the other constructors to create a new vector.

The following user-callable functions are provided for accessing the vector data arrays on the host and device and copying data between the two memory spaces. Note the generic NVECTOR operations *N_VGetArrayPointer()* and *N_VSetArrayPointer()* are mapped to the corresponding HostArray functions given below. To ensure memory coherency, a user will need to call the CopyTo or CopyFrom functions as necessary to transfer data between the host and device, unless managed (shared) memory is used.

realtype ***N_VGetHostArrayPointer_Sycl**(N_Vector v)

> This function returns a pointer to the vector host data array.

realtype ***N_VGetDeviceArrayPointer_Sycl**(N_Vector v)

> This function returns a pointer to the vector device data array.

void **N_VSetHostArrayPointer_Sycl**(realtype *h_vdata, N_Vector v)

> This function sets the host array pointer in the vector v.

void **N_VSetDeviceArrayPointer_Sycl**(realtype *d_vdata, N_Vector v)

> This function sets the device array pointer in the vector v.

void **N_VCopyToDevice_Sycl**(N_Vector v)

> This function copies host vector data to the device.

void **N_VCopyFromDevice_Sycl**(N_Vector v)

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

booleantype **N_VIsManagedMemory_Sycl**(N_Vector v)

> This function returns SUNTRUE if the vector data is allocated as managed (shared) memory otherwise it returns SUNFALSE.

The following user-callable function is provided to set the execution policies for how SYCL kernels are launched on a device.

int **N_VSetKernelExecPolicy_Sycl**(N_Vector v, *SUNSyclExecPolicy* *stream_exec_policy, *SUNSyclExecPolicy* *reduce_exec_policy)

> This function sets the execution policies which control the kernel parameters utilized when launching the streaming and reduction kernels. By default the vector is setup to use the *SUNSyclThreadDirectExecPolicy()* and

SUNSyclBlockReduceExecPolicy(). See §6.12.2 below for more information about the *SUNSyclExecPol-icy* class.

The input execution policies are cloned and, as such, may be freed after being attached to the desired vectors. A NULL input policy will reset the execution policy to the default setting.

Note: All vectors used in a single instance of a SUNDIALS package must use the same execution policy. It is **strongly recommended** that this function is called immediately after constructing the vector, and any subsequent vector be created by cloning to ensure consistent execution policies across vectors.

The following user-callable functions are provided to print the host vector data array. Unless managed memory is used, a user may need to call *N_VCopyFromDevice_Sycl()* to ensure consistency between the host and device array.

void **N_VPrint_Sycl**(N_Vector v)

This function prints the host data array to `stdout`.

void **N_VPrintFile_Sycl**(N_Vector v, FILE *outfile)

This function prints the host data array to `outfile`.

By default all fused and vector array operations are disabled in the NVECTOR_SYCL module. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with one of the above constructors, enable/disable the desired operations on that vector with the functions below, and then use this vector in conjunction with *N_VClone()* to create any additional vectors. This guarantees the new vectors will have the same operations enabled/disabled as cloned vectors inherit the same enable/disable options as the vector they are cloned from while vectors created by any of the constructors above will have the default settings for the NVECTOR_SYCL module.

int **N_VEnableFusedOps_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableLinearCombination_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableScaleAddMulti_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableLinearSumVectorArray_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableScaleVectorArray_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableConstVectorArray_Sycl**(N_Vector v, booleantype tf)

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

int **N_VEnableScaleAddMultiVectorArray_Sycl**(N_Vector v, booleantype tf)

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

---

int **N_VEnableLinearCombinationVectorArray_Sycl**(N_Vector v, booleantype tf)

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

Notes

-   When there is a need to access components of an NVECTOR_SYCL, v, it is recommended to use *N_VGetDeviceArrayPointer()* to access the device array or *N_VGetArrayPointer()* for the host array. When using managed (shared) memory, either function may be used. To ensure memory coherency, a user may need to call the CopyTo or CopyFrom functions as necessary to transfer data between the host and device, unless managed (shared) memory is used.

-   To maximize efficiency, vector operations in the NVECTOR_SYCL 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.

6.12.2 The SUNSyclExecPolicy Class

In order to provide maximum flexibility to users, the SYCL kernel execution parameters used by kernels within SUN-DIALS are defined by objects of the sundials::sycl::ExecPolicy abstract class type (this class can be accessed in the global namespace as SUNSyclExecPolicy). Thus, users may provide custom execution policies that fit the needs of their problem. The SUNSyclExecPolicy class is defined as

typedef sundials::sycl::ExecPolicy **SUNSyclExecPolicy**

where the sundials::sycl::ExecPolicy class is defined in the header file sundials_sycl_policies.hpp, as follows:

```
class ExecPolicy
{
public:
   virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const = 0;
   virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const = 0;
   virtual ExecPolicy* clone() const = 0;
   virtual ~ExecPolicy() {}
};
```

For consistency the function names and behavior mirror the execution policies for the CUDA and HIP vectors. In the SYCL case the blockSize is the local work-group range in a one-dimensional nd_range (threads per group). The gridSize is the number of local work groups so the global work-group range in a one-dimensional nd_range is blockSize * gridSize (total number of threads). All vector kernels are written with a many-to-one mapping where work units (vector elements) are mapped in a round-robin manner across the global range. As such, the blockSize and gridSize can be set to any positive value.

To define a custom execution policy, a user simply needs to create a class that inherits from the abstract class and implements the methods. The SUNDIALS provided sundials::sycl::ThreadDirectExecPolicy (aka in the global namespace as SUNSyclThreadDirectExecPolicy) class is a good example of a what a custom execution policy may look like:

```
class ThreadDirectExecPolicy : public ExecPolicy
{
public:
   ThreadDirectExecPolicy(const size_t blockDim)
      : blockDim_(blockDim)
```

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```
    {}

    ThreadDirectExecPolicy(const ThreadDirectExecPolicy& ex)
        : blockDim_(ex.blockDim_)
    {}

    virtual size_t gridSize(size_t numWorkUnits = 0, size_t blockDim = 0) const
    {
        return (numWorkUnits + blockSize() - 1) / blockSize();
    }

    virtual size_t blockSize(size_t numWorkUnits = 0, size_t gridDim = 0) const
    {
        return blockDim_;
    }

    virtual ExecPolicy* clone() const
    {
        return static_cast<ExecPolicy*>(new ThreadDirectExecPolicy(*this));
    }

private:
    const size_t blockDim_;
};
```

SUNDIALS provides the following execution policies:

SUNSyclThreadDirectExecPolicy(const size_t blockDim)

> Is for kernels performing streaming operations and maps each work unit (vector element) to a work-item (thread). Based on the local work-group range (number of threads per group, `blockSize`) the number of local work-groups (`gridSize`) is computed so there are enough work-items in the global work-group range (total number of threads, `blockSize * gridSize`) for one work unit per work-item (thread).

SUNSyclGridStrideExecPolicy(const size_t blockDim, const size_t gridDim)

> Is for kernels performing streaming operations and maps each work unit (vector element) to a work-item (thread) in a round-robin manner so the local work-group range (number of threads per group, `blockSize`) and the number of local work-groups (`gridSize`) can be set to any positive value. In this case the global work-group range (total number of threads, `blockSize * gridSize`) may be less than the number of work units (vector elements).

SUNSyclBlockReduceExecPolicy(const size_t blockDim)

> Is for kernels performing a reduction, the local work-group range (number of threads per group, `blockSize`) and the number of local work-groups (`gridSize`) can be set to any positive value or the `gridSize` may be set to `0` in which case the global range is chosen so that there are enough threads for at most two work units per work-item.

By default the NVECTOR_SYCL module uses the SUNSyclThreadDirectExecPolicy and SUNSyclBlockReduce-ExecPolicy where the default `blockDim` is determined by querying the device for the `max_work_group_size`. User may specify different policies by constructing a new SyclExecPolicy and attaching it with *N_VSetKernelExecPolicy_Sycl()*. For example, a policy that uses 128 work-items (threads) per group can be created and attached like so:

```
N_Vector v = N_VNew_Sycl(length, SUNContext sunctx);
SUNSyclThreadDirectExecPolicy thread_direct(128);
```

```
SUNSyclBlockReduceExecPolicy  block_reduce(128);
flag = N_VSetKernelExecPolicy_Sycl(v, &thread_direct, &block_reduce);
```

These default policy objects can be reused for multiple SUNDIALS data structures (e.g. a *SUNMatrix* and an *N_-Vector*) since they do not hold any modifiable state information.

6.13 The NVECTOR_RAJA Module

The NVECTOR_RAJA module is an experimental NVECTOR implementation using the RAJA hardware abstraction layer. In this implementation, RAJA allows for SUNDIALS vector kernels to run on AMD, NVIDIA, or Intel GPU devices. The module is intended for users who are already familiar with RAJA and GPU programming. Building this vector module requires a C++11 compliant compiler and either the NVIDIA CUDA programming environment, the AMD ROCm HIP programming environment, or a compiler that supports the SYCL abstraction layer. When using the AMD ROCm HIP environment, the HIP-clang compiler must be utilized. Users can select which backend to compile with by setting the `SUNDIALS_RAJA_BACKENDS` CMake variable to either CUDA, HIP, or SYCL. Besides the CUDA, HIP, and SYCL backends, RAJA has other backends such as serial, OpenMP, and OpenACC. These backends are not used in this SUNDIALS release.

The vector content layout is as follows:

```
struct _N_VectorContent_Raja
{
    sunindextype length;
    booleantype  own_data;
    realtype*    host_data;
    realtype*    device_data;
    void*        priv; /* 'private' data */
};
```

The content members are the vector length (size), a boolean flag that signals if the vector owns the data (i.e., it is in charge of freeing the data), pointers to vector data on the host and the device, and a private data structure which holds the memory management type, which should not be accessed directly.

When instantiated with *N_VNew_Raja()*, the underlying data will be allocated on both the host and the device. Alternatively, a user can provide host and device data arrays by using the *N_VMake_Raja()* constructor. To use managed memory, the constructors *N_VNewManaged_Raja()* and *N_VMakeManaged_Raja()* are provided. Details on each of these constructors are provided below.

The header file to include when using this is `nvector_raja.h`. The installed module library to link to is `libsundials_nveccudaraja.lib` when using the CUDA backend, `libsundials_nvechipraja.lib` when using the HIP backend, and `libsundials_nvecsyclraja.lib` when using the SYCL backend. The extension `.lib` is typically `.so` for shared libraries `.a` for static libraries.

6.13.1 NVECTOR_RAJA functions

Unlike other native SUNDIALS vector types, the NVECTOR_RAJA module does not provide macros to access its member variables. Instead, user should use the accessor functions:

realtype ***N_VGetHostArrayPointer_Raja**(*N_Vector* v)

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

realtype ***N_VGetDeviceArrayPointer_Raja**(*N_Vector* v)

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

booleantype **N_VIsManagedMemory_Raja**(*N_Vector* v)

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

The NVECTOR_RAJA module defines the implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VDotProdMulti()*, *N_VWrmsNormVectorArray()*, and *N_VWrmsNormMaskVectorArray()* as support for arrays of reduction vectors is not yet supported in RAJA. These functions will be added to the NVECTOR_RAJA implementation in the future. Additionally, the operations *N_VGetArrayPointer()* and *N_VSetArrayPointer()* are not implemented by the RAJA vector. As such, this vector cannot be used with SUNDIALS direct solvers and preconditioners. The NVECTOR_RAJA module provides separate functions to access data on the host and on the device. It also provides methods for copying from the host to the device and vice versa. Usage examples of NVECTOR_RAJA are provided in some example programs for CVODE [40].

The names of vector operations are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffix `_Raja` (e.g. `N_VDestroy_Raja`). The module NVECTOR_RAJA provides the following additional user-callable routines:

N_Vector **N_VNew_Raja**(*sunindextype* vec_length, *SUNContext* sunctx)

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

N_Vector **N_VNewManaged_Raja**(*sunindextype* vec_length, *SUNContext* sunctx)

> This function creates and allocates memory for a RAJA `N_Vector`. The vector data array is allocated in managed memory.

N_Vector **N_VMake_Raja**(*sunindextype* length, *realtype* *h_data, *realtype* *v_data, *SUNContext* sunctx)

> This function creates an NVECTOR_RAJA with user-supplied host and device data arrays. This function does not allocate memory for data itself.

N_Vector **N_VMakeManaged_Raja**(*sunindextype* length, *realtype* *vdata, *SUNContext* sunctx)

> This function creates an NVECTOR_RAJA with a user-supplied managed memory data array. This function does not allocate memory for data itself.

N_Vector **N_VNewWithMemHelp_Raja**(*sunindextype* length, *booleantype* use_managed_mem, *SUNMemoryHelper* helper, *SUNContext* sunctx)

> This function creates an NVECTOR_RAJA with a user-supplied SUNMemoryHelper for allocating/freeing memory.

N_Vector **N_VNewEmpty_Raja**()

> This function creates a new `N_Vector` where the members of the content structure have not been allocated. This utility function is used by the other constructors to create a new vector.

void **N_VCopyToDevice_Raja**(*N_Vector* v)

> This function copies host vector data to the device.

void **N_VCopyFromDevice_Raja**(*N_Vector* v)

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

void **N_VPrint_Raja**(*N_Vector* v)

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

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

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

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

int **N_VEnableFusedOps_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_Raja**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_Raja**(*N_Vector* v, *booleantype* tf)

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

Notes

- When there is a need to access components of an NVECTOR_RAJA vector, it is recommended to use functions *N_VGetDeviceArrayPointer_Raja()* or *N_VGetHostArrayPointer_Raja()*. However, when using managed memory, the function *N_VGetArrayPointer()* may also be used.

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

6.14 The NVECTOR_KOKKOS Module

New in version 6.4.0.

The NVECTOR_KOKKOS *N_Vector* implementation provides a vector data structure using Kokkos [28, 55] to support a variety of backends including serial, OpenMP, CUDA, HIP, and SYCL. Since Kokkos is a modern C++ library, the module is also written in modern C++ (it requires C++14) as a header only library. To utilize this N_Vector users will need to include nvector/nvector_kokkos.hpp. More instructions on building SUNDIALS with Kokkos enabled are given in §11.1.4. For instructions on building and using Kokkos, refer to the Kokkos documentation.

6.14.1 Using NVECTOR_KOKKOS

The NVECTOR_KOKKOS module is defined by the Vector templated class in the sundials::kokkos namespace:

```
template<class ExecutionSpace = Kokkos::DefaultExecutionSpace,
         class MemorySpace = typename ExecutionSpace::memory_space>
   class Vector : public sundials::impl::BaseNVector,
                  public sundials::ConvertibleTo<N_Vector>
```

To use the NVECTOR_KOKKOS module, we construct an instance of the Vector class e.g.,

```
// Vector with extent length using the default execution space
sundials::kokkos::Vector<> x{length, sunctx};

// Vector with extent length using the Cuda execution space
sundials::kokkos::Vector<Kokkos::Cuda> x{length, sunctx};

// Vector based on an existing Kokkos::View
Kokkos::View<> view{"a view", length};
sundials::kokkos::Vector<> x{view, sunctx};

// Vector based on an existing Kokkos::View for device and host
Kokkos::View<Kokkos::Cuda> device_view{"a view", length};
Kokkos::View<Kokkos::HostMirror> host_view{Kokkos::create_mirror_view(device_view)};
sundials::kokkos::Vector<> x{device_view, host_view, sunctx};
```

Instances of the Vector class are implicitly or explicitly (using the *Convert()* method) convertible to a *N_Vector* e.g.,

```
sundials::kokkos::Vector<> x{length, sunctx};
N_Vector x2 = x;            // implicit conversion to N_Vector
N_Vector x3 = x.Convert(); // explicit conversion to N_Vector
```

No further interaction with a Vector is required from this point, and it is possible to use the *N_Vector* API to operate on x2 or x3.

> **Warning:** *N_VDestroy()* should never be called on a N_Vector that was created via conversion from a sundials::kokkos::Vector. Doing so may result in a double free.

The underlying Vector can be extracted from a N_Vector using *GetVec()* e.g.,

```
auto x_vec = GetVec<>(x3);
```

6.14.2 NVECTOR_KOKKOS API

In this section we list the public API of the `sundials::kokkos::Vector` class.

template<class **ExecutionSpace** = Kokkos::DefaultExecutionSpace, class **MemorySpace** = class *ExecutionSpace*::memory_space>

class **Vector** : public sundials::impl::BaseNVector, public sundials::ConvertibleTo<N_Vector>

> **Vector**() = default
>
>> Default constructor – the vector must be copied or moved to.
>
> **Vector**(size_type length, SUNContext sunctx)
>
>> Constructs a single `Vector` which is based on a 1D `Kokkos::View` with the ExecutionSpace and MemorySpace provided as template arguments.
>>
>>> **Parameters**
>>>
>>> - **length** – length of the vector (i.e., the extent of the View)
>>> - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **Vector**(view_type view, SUNContext sunctx)
>
>> Constructs a single `Vector` from an existing `Kokkos::View`. The View ExecutionSpace and MemorySpace must match the ExecutionSpace and MemorySpace provided as template arguments.
>>
>>> **Parameters**
>>>
>>> - **view** – A 1D `Kokkos::View`
>>> - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **Vector**(view_type view, host_view_type host_view, SUNContext sunctx)
>
>> Constructs a single `Vector` from an existing `Kokkos::View` for the device and the host. The ExecutionSpace and MemorySpace of the device View must match the ExecutionSpace and MemorySpace provided as template arguments.
>>
>>> **Parameters**
>>>
>>> - **view** – A 1D `Kokkos::View` for the device
>>> - **host_view** – A 1D `Kokkos::View` that is a `Kokkos::HostMirrror` for the device view
>>> - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **Vector**(*Vector* &&that_vector) noexcept
>
>> Move constructor.
>
> **Vector**(const *Vector* &that_vector)
>
>> Copy constructor. This creates a clone of the Vector, i.e., it creates a new Vector with the same properties, such as length, but it does not copy the data.
>
> *Vector* &**operator=**(*Vector* &&rhs) noexcept
>
>> Move assignment.
>
> *Vector* &**operator=**(const *Vector* &rhs)
>
>> Copy assignment. This creates a clone of the Vector, i.e., it creates a new Vector with the same properties, such as length, but it does not copy the data.
>
> virtual **~Vector**() = default;
>
>> Default destructor.

size_type **Length**()
>   Get the vector length i.e., `extent(0)`.

view_type **View**()
>   Get the underlying `Kokkos:View` for the device.

host_view_type **HostView**()
>   Get the underlying `Kokkos:View` for the host.

operator N_Vector() override
>   Implicit conversion to a *N_Vector*.

operator N_Vector() const override
>   Implicit conversion to a *N_Vector*.

N_Vector **Convert**() override
>   Explicit conversion to a *N_Vector*.

N_Vector **Convert**() const override
>   Explicit conversion to a *N_Vector*.

template<class **VectorType**>
inline *VectorType* ***GetVec**(N_Vector v)
>   Get the *Vector* wrapped by a *N_Vector*.

void **CopyToDevice**(N_Vector v)
>   Copy the data from the host view to the device view with `Kokkos::deep_copy`.

void **CopyFromDevice**(N_Vector v)
>   Copy the data to the host view from the device view with `Kokkos::deep_copy`.

template<class **VectorType**>
void **CopyToDevice**(*VectorType* &v)
>   Copy the data from the host view to the device view with `Kokkos::deep_copy`.

template<class **VectorType**>
void **CopyFromDevice**(*VectorType* &v)
>   Copy the data to the host view from the device view with `Kokkos::deep_copy`.

6.15 The NVECTOR_OPENMPDEV Module

In situations where a user has access to a device such as a GPU for offloading computation, SUNDIALS provides an NVECTOR implementation using OpenMP device offloading, called NVECTOR_OPENMPDEV.

The NVECTOR_OPENMPDEV implementation defines the *content* field of the `N_Vector` to be a structure containing the length of the vector, a pointer to the beginning of a contiguousdata array on the host, a pointer to the beginning of a contiguous data array on the device, and a boolean flag `own_data` which specifies the ownership of host and device data arrays.

```
struct _N_VectorContent_OpenMPDEV
{
  sunindextype length;
  booleantype  own_data;
  realtype     *host_data;
  realtype     *dev_data;
};
```

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

6.15.1 NVECTOR_OPENMPDEV accessor macros

The following macros are provided to access the content of an NVECTOR_OPENMPDEV vector.

NV_CONTENT_OMPDEV(v)

This macro gives access to the contents of the NVECTOR_OPENMPDEV `N_Vector v`.

The assignment `v_cont = NV_CONTENT_S(v)` sets `v_cont` to be a pointer to the NVECTOR_OPENMPDEV content structure.

Implementation:

```
#define NV_CONTENT_OMPDEV(v) ( (N_VectorContent_OpenMPDEV)(v->content) )
```

NV_OWN_DATA_OMPDEV(v)

Access the *own_data* component of the OpenMPDEV `N_Vector v`.

The assignment `v_data = NV_DATA_HOST_OMPDEV(v)` sets `v_data` to be a pointer to the first component of the data on the host for the `N_Vector v`.

Implementation:

```
#define NV_OWN_DATA_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->own_data )
```

NV_DATA_HOST_OMPDEV(v)

The assignment `NV_DATA_HOST_OMPDEV(v) = v_data` sets the host component array of `v` to be `v_data` by storing the pointer `v_data`.

Implementation:

```
#define NV_DATA_HOST_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->host_data )
```

NV_DATA_DEV_OMPDEV(v)

The assignment `v_dev_data = NV_DATA_DEV_OMPDEV(v)` sets `v_dev_data` to be a pointer to the first component of the data on the device for the `N_Vector v`. The assignment `NV_DATA_DEV_OMPDEV(v) = v_dev_data` sets the device component array of `v` to be `v_dev_data` by storing the pointer `v_dev_data`.

Implementation:

```
#define NV_DATA_DEV_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->dev_data )
```

NV_LENGTH_OMPDEV(V)

Access the *length* component of the OpenMPDEV `N_Vector v`.

The assignment `v_len = NV_LENGTH_OMPDEV(v)` sets `v_len` to be the length of `v`. On the other hand, the call `NV_LENGTH_OMPDEV(v) = len_v` sets the length of `v` to be `len_v`.

```
#define NV_LENGTH_OMPDEV(v) ( NV_CONTENT_OMPDEV(v)->length )
```

6.15.2 NVECTOR_OPENMPDEV functions

The NVECTOR_OPENMPDEV module defines OpenMP device offloading implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VSetArrayPointer()*. As such, this vector cannot be used with the SUNDIALS direct solvers and preconditioners. It also provides methods for copying from the host to the device and vice versa.

The names of the vector operations are obtained from those in §6.2, §6.2.2, §6.2.3, and §6.2.4 by appending the suffix _OpenMPDEV (e.g. N_VDestroy_OpenMPDEV). The module NVECTOR_OPENMPDEV provides the following additional user-callable routines:

N_Vector **N_VNew_OpenMPDEV**(*sunindextype* vec_length, *SUNContext* sunctx)

>   This function creates and allocates memory for an NVECTOR_OPENMPDEV N_Vector.

N_Vector **N_VNewEmpty_OpenMPDEV**(*sunindextype* vec_length, *SUNContext* sunctx)

>   This function creates a new NVECTOR_OPENMPDEV N_Vector with an empty (NULL) data array.

N_Vector **N_VMake_OpenMPDEV**(*sunindextype* vec_length, *realtype* *h_vdata, *realtype* *d_vdata, *SUNContext* sunctx)

>   This function creates an NVECTOR_OPENMPDEV vector with user-supplied vector data arrays h_vdata and d_vdata. This function does not allocate memory for data itself.

realtype ***N_VGetHostArrayPointer_OpenMPDEV**(*N_Vector* v)

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

realtype ***N_VGetDeviceArrayPointer_OpenMPDEV**(*N_Vector* v)

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

void **N_VPrint_OpenMPDEV**(*N_Vector* v)

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

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

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

void **N_VCopyToDevice_OpenMPDEV**(*N_Vector* v)

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

void **N_VCopyFromDevice_OpenMPDEV**(*N_Vector* v)

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

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

int **N_VEnableFusedOps_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMultiVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombinationVectorArray_OpenMPDEV**(*N_Vector* v, *booleantype* tf)

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

Notes

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

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

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

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

6.16 The NVECTOR_TRILINOS Module

The NVECTOR_TRILINOS module is an NVECTOR wrapper around the Trilinos Tpetra vector. The interface to Tpetra is implemented in the `sundials::trilinos::nvector_tpetra::TpetraVectorInterface` class. This class simply stores a reference counting pointer to a Tpetra vector and inherits from an empty structure

```
struct _N_VectorContent_Trilinos {};
```

to interface the C++ class with the NVECTOR C code. A pointer to an instance of this class is kept in the *content* field of the `N_Vector` object, to ensure that the Tpetra vector is not deleted for as long as the `N_Vector` object exists.

The Tpetra vector type in the `sundials::trilinos::nvector_tpetra::TpetraVectorInterface` class is defined as:

typedef Tpetra::Vector<realtype, int, sunindextype> **vector_type**;

The Tpetra vector will use the SUNDIALS-specified `realtype` as its scalar type, `int` as the local ordinal type, and `sunindextype` as the global ordinal type. This type definition will use Tpetra's default node type. Available Kokkos node types as of the Trilinos 12.14 release are serial (single thread), OpenMP, Pthread, and CUDA. The default node type is selected when building the Kokkos package. For example, the Tpetra vector will use a CUDA node if Tpetra was built with CUDA support and the CUDA node was selected as the default when Tpetra was built.

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

6.16.1 NVECTOR_TRILINOS functions

The NVECTOR_TRILINOS module defines implementations of all vector operations listed in §6.2, §6.2.2, §6.2.3, and §6.2.4, except for *N_VGetArrayPointer()* and *N_VSetArrayPointer()*. As such, this vector cannot be used with the SUNDIALS direct solvers and preconditioners. When access to raw vector data is needed, it is recommended to extract the Trilinos Tpetra vector first, and then use Tpetra vector methods to access the data. Usage examples of NVECTOR_TRILINOS are provided in example programs for IDA.

The names of vector operations are obtained from those in §6.2 by appending the suffice _Trilinos (e.g. N_VDestroy_Trilinos). Vector operations call existing `Tpetra::Vector` methods when available. Vector operations specific to SUNDIALS are implemented as standalone functions in the namespace `sundials::trilinos::nvector_tpetra::TpetraVector`, located in the file `SundialsTpetraVectorKernels.hpp`. The module NVECTOR_TRILINOS provides the following additional user-callable routines:

Teuchos::RCP<*vector_type*> **N_VGetVector_Trilinos**(N_Vector v)

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

N_Vector **N_VMake_Trilinos**(Teuchos::RCP<*vector_type*> v)

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

Notes

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

```
typedef sundials::trilinos::nvector_tpetra::TpetraVectorInterface::vector_type vector_type
```

> This will ensure that data types used in Tpetra vector match those in SUNDIALS.

- When there is a need to access components of an `N_Vector_Trilinos` v, it is recommeded to extract the Trilinos vector object via `x_vec = N_VGetVector_Trilinos(v)` and then access components using the appropriate Trilinos functions.

- The functions `N_VDestroy_Trilinos` and `N_VDestroyVectorArray_Trilinos` only delete the `N_Vector` wrapper. The underlying Tpetra vector object will exist for as long as there is at least one reference to it.

6.17 The NVECTOR_MANYVECTOR Module

The NVECTOR_MANYVECTOR module is designed to facilitate problems with an inherent data partitioning within a computational node for the solution vector. These data partitions are entirely user-defined, through construction of distinct NVECTOR modules for each component, that are then combined together to form the NVECTOR_MANYVECTOR. Two potential use cases for this flexibility include:

A. *Heterogenous computational architectures*: for data partitioning between different computing resources on a node, architecture-specific subvectors may be created for each partition. For example, a user could create one GPU-accelerated component based on *NVECTOR_CUDA*, and another CPU threaded component based on *NVECTOR_OPENMP*.

B. *Structure of arrays (SOA) data layouts*: for problems that require separate subvectors for each solution component. For example, in an incompressible Navier-Stokes simulation, separate subvectors may be used for velocities and pressure, which are combined together into a single NVECTOR_MANYVECTOR for the overall "solution".

The above use cases are neither exhaustive nor mutually exclusive, and the NVECTOR_MANYVECTOR implementation should support arbitrary combinations of these cases.

The NVECTOR_MANYVECTOR implementation is designed to work with any NVECTOR subvectors that implement the minimum "standard" set of operations in §6.2.1. Additionally, NVECTOR_MANYVECTOR sets no limit on the number of subvectors that may be attached (aside from the limitations of using `sunindextype` for indexing, and standard per-node memory limitations). However, while this ostensibly supports subvectors with one entry each (i.e., one subvector for each solution entry), we anticipate that this extreme situation will hinder performance due to non-stride-one memory accesses and increased function call overhead. We therefore recommend a relatively coarse partitioning of the problem, although actual performance will likely be problem-dependent.

As a final note, in the coming years we plan to introduce additional algebraic solvers and time integration modules that will leverage the problem partitioning enabled by NVECTOR_MANYVECTOR. However, even at present we anticipate that users will be able to leverage such data partitioning in their problem-defining ODE right-hand side function, DAE or nonlinear solver residual function, preconditioners, or custom *SUNLinearSolver* or *SUNNonlinearSolver* modules.

6.17.1 NVECTOR_MANYVECTOR structure

The NVECTOR_MANYVECTOR implementation defines the *content* field of `N_Vector` to be a structure containing the number of subvectors comprising the ManyVector, the global length of the ManyVector (including all subvectors), a pointer to the beginning of the array of subvectors, and a boolean flag `own_data` indicating ownership of the subvectors that populate `subvec_array`.

```
struct _N_VectorContent_ManyVector {
  sunindextype  num_subvectors;  /* number of vectors attached    */
  sunindextype  global_length;   /* overall manyvector length     */
  N_Vector*     subvec_array;    /* pointer to N_Vector array     */
  booleantype   own_data;        /* flag indicating data ownership */
};
```

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

6.17.2 NVECTOR_MANYVECTOR functions

The NVECTOR_MANYVECTOR module implements all vector operations listed in §6.2 except for *N_VGetArray-Pointer()*, *N_VSetArrayPointer()*, *N_VScaleAddMultiVectorArray()*, and *N_VLinearCombinationVec-torArray()*. As such, this vector cannot be used with the SUNDIALS direct solvers and preconditioners. Instead, the NVECTOR_MANYVECTOR module provides functions to access subvectors, whose data may in turn be accessed according to their NVECTOR implementations.

The names of vector operations are obtained from those in §6.2 by appending the suffix `_ManyVector` (e.g. `N_-VDestroy_ManyVector`). The module NVECTOR_MANYVECTOR provides the following additional user-callable routines:

N_Vector **N_VNew_ManyVector**(*sunindextype* num_subvectors, *N_Vector* *vec_array, *SUNContext* sunctx)

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

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

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

    Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions *N_VNewVectorArray()*, and *N_VSetVecAtIndexVectorArray()* to create the `N_Vector*` argument. This is further explained in §4.5.2.5, and the functions are documented in §6.1.1.

N_Vector **N_VGetSubvector_ManyVector**(*N_Vector* v, *sunindextype* vec_num)

    This function returns the *vec_num* subvector from the NVECTOR array.

sunindextype **N_VGetSubvectorLocalLength_ManyVector**(*N_Vector* v, *sunindextype* vec_num)

    This function returns the local length of the *vec_num* subvector from the NVECTOR array.

    Usage:

```
local_length = N_VGetSubvectorLocalLength_ManyVector(v, 0);
```

realtype ***N_VGetSubvectorArrayPointer_ManyVector**(*N_Vector* v, *sunindextype* vec_num)

    This function returns the data array pointer for the *vec_num* subvector from the NVECTOR array.

If the input *vec_num* is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then NULL is returned.

int **N_VSetSubvectorArrayPointer_ManyVector**(*realtype* *v_data, *N_Vector* v, *sunindextype* vec_num)

This function sets the data array pointer for the *vec_num* subvector from the NVECTOR array.

If the input *vec_num* is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then `-1` is returned; otherwise it returns `0`.

sunindextype **N_VGetNumSubvectors_ManyVector**(*N_Vector* v)

This function returns the overall number of subvectors in the ManyVector object.

By default all fused and vector array operations are disabled in the NVECTOR_MANYVECTOR module, except for *N_VWrmsNormVectorArray()* and *N_VWrmsNormMaskVectorArray()*, that are enabled by default. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with *N_VNew_ManyVector()*, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using *N_VClone()*. This guarantees that the new vectors will have the same operations enabled/disabled, since cloned vectors inherit those configuration options from the vector they are cloned from, while vectors created with *N_VNew_ManyVector()* will have the default settings for the NVECTOR_MANYVECTOR module. We note that these routines *do not* call the corresponding routines on subvectors, so those should be set up as desired *before* attaching them to the ManyVector in *N_VNew_ManyVector()*.

int **N_VEnableFusedOps_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_ManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_ManyVector**(*N_Vector* v, *booleantype* tf)

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

Notes

- *N_VNew_ManyVector()* sets the field `own_data = SUNFALSE`. N_VDestroy_ManyVector() will not attempt to call *N_VDestroy()* on any subvectors contained in the subvector array for any N_Vector with `own_data` set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the subvectors.

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

6.18 The NVECTOR_MPIMANYVECTOR Module

The NVECTOR_MPIMANYVECTOR module is designed to facilitate problems with an inherent data partitioning for the solution vector, and when using distributed-memory parallel architectures. As such, this implementation supports all use cases allowed by the MPI-unaware NVECTOR_MANYVECTOR implementation, as well as partitioning data between nodes in a parallel environment. These data partitions are entirely user-defined, through construction of distinct NVECTOR modules for each component, that are then combined together to form the NVECTOR_MPIMANYVECTOR. Three potential use cases for this module include:

A. *Heterogenous computational architectures (single-node or multi-node)*: for data partitioning between different computing resources on a node, architecture-specific subvectors may be created for each partition. For example, a user could create one MPI-parallel component based on *NVECTOR_PARALLEL*, another GPU-accelerated component based on *NVECTOR_CUDA*.

B. *Process-based multiphysics decompositions (multi-node)*: for computations that combine separate MPI-based simulations together, each subvector may reside on a different MPI communicator, and the MPIManyVector combines these via an MPI *intercommunicator* that connects these distinct simulations together.

C. *Structure of arrays (SOA) data layouts (single-node or multi-node)*: for problems that require separate subvectors for each solution component. For example, in an incompressible Navier-Stokes simulation, separate subvectors may be used for velocities and pressure, which are combined together into a single MPIManyVector for the overall "solution".

The above use cases are neither exhaustive nor mutually exclusive, and the NVECTOR_MANYVECTOR implementation should support arbitrary combinations of these cases.

The NVECTOR_MPIMANYVECTOR implementation is designed to work with any NVECTOR subvectors that implement the minimum "standard" set of operations in §6.2.1, however significant performance benefits may be obtained when subvectors additionally implement the optional local reduction operations listed in §6.2.4.

Additionally, NVECTOR_MPIMANYVECTOR sets no limit on the number of subvectors that may be attached (aside from the limitations of using `sunindextype` for indexing, and standard per-node memory limitations). However, while this ostensibly supports subvectors with one entry each (i.e., one subvector for each solution entry), we anticipate that this extreme situation will hinder performance due to non-stride-one memory accesses and increased function call overhead. We therefore recommend a relatively coarse partitioning of the problem, although actual performance will likely be problem-dependent.

As a final note, in the coming years we plan to introduce additional algebraic solvers and time integration modules that will leverage the problem partitioning enabled by NVECTOR_MPIMANYVECTOR. However, even at present we anticipate that users will be able to leverage such data partitioning in their problem-defining ODE right-hand side function, DAE or nonlinear solver residual function, preconditioners, or custom *SUNLinearSolver* or *SUNNonlinearSolver* modules.

6.18.1 NVECTOR_MPIMANYVECTOR structure

The NVECTOR_MPIMANYVECTOR implementation defines the *content* field of `N_Vector` to be a structure containing the MPI communicator (or `MPI_COMM_NULL` if running on a single-node), the number of subvectors comprising the MPIManyVector, the global length of the MPIManyVector (including all subvectors on all MPI ranks), a pointer to the beginning of the array of subvectors, and a boolean flag `own_data` indicating ownership of the subvectors that populate `subvec_array`.

```
struct _N_VectorContent_MPIManyVector {
  MPI_Comm      comm;            /* overall MPI communicator      */
  sunindextype  num_subvectors;  /* number of vectors attached    */
  sunindextype  global_length;   /* overall mpimanyvector length   */
  N_Vector*     subvec_array;    /* pointer to N_Vector array      */
  booleantype   own_data;        /* flag indicating data ownership */
};
```

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

Note: If SUNDIALS is configured with MPI disabled, then the MPIManyVector library will not be built. Furthermore, any user codes that include `nvector_mpimanyvector.h` *must* be compiled using an MPI-aware compiler (whether the specific user code utilizes MPI or not). We note that the NVECTOR_MANYVECTOR implementation is designed for ManyVector use cases in an MPI-unaware environment.

6.18.2 NVECTOR_MPIMANYVECTOR functions

The NVECTOR_MPIMANYVECTOR module implements all vector operations listed in §6.2, except for *N_VGetArrayPointer()*, *N_VSetArrayPointer()*, *N_VScaleAddMultiVectorArray()*, and *N_VLinearCombinationVectorArray()*. As such, this vector cannot be used with the SUNDIALS direct solvers and preconditioners. Instead, the NVECTOR_MPIMANYVECTOR module provides functions to access subvectors, whose data may in turn be accessed according to their NVECTOR implementations.

The names of vector operations are obtained from those in §6.2 by appending the suffix `_MPIManyVector` (e.g. `N_VDestroy_MPIManyVector`). The module NVECTOR_MPIMANYVECTOR provides the following additional usercallable routines:

N_Vector **N_VNew_MPIManyVector**(*sunindextype* num_subvectors, *N_Vector* *vec_array, *SUNContext* sunctx)

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

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

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

> Users of the Fortran 2003 interface to this function will first need to use the generic `N_Vector` utility functions *N_VNewVectorArray()*, and *N_VSetVecAtIndexVectorArray()* to create the `N_Vector*` argument. This is further explained in §4.5.2.5, and the functions are documented in §6.1.1.

N_Vector **N_VMake_MPIManyVector**(MPI_Comm comm, *sunindextype* num_subvectors, *N_Vector* *vec_array, *SUNContext* sunctx)

> This function creates a MPIManyVector from a set of existing NVECTOR objects, and a user-created MPI communicator that "connects" these subvectors. Any MPI-aware subvectors may use different MPI communicators than the input *comm*. We note that this routine is designed to support any combination of the use cases above.

> The input *comm* should be this user-created MPI communicator. This routine will internally call `MPI_Comm_dup` to create a copy of the input `comm`, so the user-supplied `comm` argument need not be retained after the call to `N_VMake_MPIManyVector()`.

> If all subvectors are MPI-unaware, then the input *comm* argument should be `MPI_COMM_NULL`, although in this case, it would be simpler to call `N_VNew_MPIManyVector()` instead, or to just use the NVECTOR_MANYVECTOR module.

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

> Upon successful completion, the new MPIManyVector is returned; otherwise this routine returns `NULL` (e.g., if the input *vec_array* is NULL).

N_Vector **N_VGetSubvector_MPIManyVector**(*N_Vector* v, *sunindextype* vec_num)

> This function returns the *vec_num* subvector from the NVECTOR array.

sunindextype **N_VGetSubvectorLocalLength_MPIManyVector**(*N_Vector* v, *sunindextype* vec_num)

> This function returns the local length of the *vec_num* subvector from the NVECTOR array.

> Usage:

```
local_length = N_VGetSubvectorLocalLength_MPIManyVector(v, 0);
```

realtype ****N_VGetSubvectorArrayPointer_MPIManyVector**(*N_Vector* v, *sunindextype* vec_num)

> This function returns the data array pointer for the *vec_num* subvector from the NVECTOR array.

> If the input *vec_num* is invalid, or if the subvector does not support the `N_VGetArrayPointer` operation, then `NULL` is returned.

int **N_VSetSubvectorArrayPointer_MPIManyVector**(*realtype* *v_data, *N_Vector* v, *sunindextype* vec_num)

> This function sets the data array pointer for the *vec_num* subvector from the NVECTOR array.

> If the input *vec_num* is invalid, or if the subvector does not support the `N_VSetArrayPointer` operation, then `-1` is returned; otherwise it returns `0`.

sunindextype **N_VGetNumSubvectors_MPIManyVector**(*N_Vector* v)

> This function returns the overall number of subvectors in the MPIManyVector object.

By default all fused and vector array operations are disabled in the NVECTOR_MPIMANYVECTOR module, except for `N_VWrmsNormVectorArray()` and `N_VWrmsNormMaskVectorArray()`, that are enabled by default. The following additional user-callable routines are provided to enable or disable fused and vector array operations for a specific vector. To ensure consistency across vectors it is recommended to first create a vector with `N_VNew_MPIManyVector()` or `N_VMake_MPIManyVector()`, enable/disable the desired operations for that vector with the functions below, and create any additional vectors from that vector using `N_VClone()`. This guarantees that the new vectors will have the same operations enabled/disabled, since cloned vectors inherit those configuration options from the vector they are cloned from, while vectors created with `N_VNew_MPIManyVector()` and `N_VMake_MPIManyVector()` will have the default settings for the NVECTOR_MPIMANYVECTOR module. We note that these routines *do not* call the corresponding routines on subvectors, so those should be set up as desired *before* attaching them to the MPIManyVector in `N_VNew_MPIManyVector()` or `N_VMake_MPIManyVector()`.

int **N_VEnableFusedOps_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearCombination_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleAddMulti_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableDotProdMulti_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableLinearSumVectorArray_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableScaleVectorArray_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableConstVectorArray_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormVectorArray_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

int **N_VEnableWrmsNormMaskVectorArray_MPIManyVector**(*N_Vector* v, *booleantype* tf)

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

Notes

- *N_VNew_MPIManyVector()* and *N_VMake_MPIManyVector()* set the field `own_data = SUNFALSE`. N_VDestroy_MPIManyVector() will not attempt to call *N_VDestroy()* on any subvectors contained in the subvector array for any `N_Vector` with `own_data` set to SUNFALSE. In such a case, it is the user's responsibility to deallocate the subvectors.

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

6.19 The NVECTOR_MPIPLUSX Module

The NVECTOR_MPIPLUSX module is designed to facilitate the MPI+X paradigm, where X is some form of on-node (local) parallelism (e.g. OpenMP, CUDA). This paradigm is becoming increasingly popular with the rise of heterogeneous computing architectures.

The NVECTOR_MPIPLUSX implementation is designed to work with any NVECTOR that implements the minimum "standard" set of operations in §6.2.1. However, it is not recommended to use the NVECTOR_PARALLEL, NVEC-TOR_PARHYP, NVECTOR_PETSC, or NVECTOR_TRILINOS implementations underneath the NVECTOR_MPI-PLUSX module since they already provide MPI capabilities.

6.19.1 NVECTOR_MPIPLUSX structure

The NVECTOR_MPIPLUSX implementation is a thin wrapper around the NVECTOR_MPIMANYVECTOR. Accordingly, it adopts the same content structure as defined in §6.18.1.

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

Note: If SUNDIALS is configured with MPI disabled, then the mpiplusx library will not be built. Furthermore, any user codes that include `nvector_mpiplusx.h` *must* be compiled using an MPI-aware compiler.

6.19.2 NVECTOR_MPIPLUSX functions

The NVECTOR_MPIPLUSX module adopts all vector operations listed in §6.2, from the NVECTOR_MPI-MANYVECTOR (see §6.18) except for *N_VGetArrayPointer()*, and *N_VSetArrayPointer()*; the module provides its own implementation of these functions that call the local vector implementations. Therefore, the NVECTOR_-MPIPLUSX module implements all of the operations listed in the referenced sections except for *N_VScaleAddMultiVectorArray()*, and *N_VLinearCombinationVectorArray()*. Accordingly, it's compatibility with the SUNDI-ALS direct solvers and preconditioners depends on the local vector implementation.

The module NVECTOR_MPIPLUSX provides the following additional user-callable routines:

N_Vector **N_VMake_MPIPlusX**(MPI_Comm comm, *N_Vector* *local_vector, *SUNContext* sunctx)

> This function creates a MPIPlusX vector from an exisiting local (i.e. on node) NVECTOR object, and a user-created MPI communicator.
>
> The input *comm* should be this user-created MPI communicator. This routine will internally call `MPI_Comm_dup` to create a copy of the input `comm`, so the user-supplied `comm` argument need not be retained after the call to *N_VMake_MPIPlusX()*.
>
> This routine will copy the NVECTOR pointer to the input `local_vector`, so the underlying local NVECTOR object should not be destroyed before the mpiplusx that contains it.
>
> Upon successful completion, the new MPIPlusX is returned; otherwise this routine returns NULL (e.g., if the input *local_vector* is NULL).

N_Vector **N_VGetLocalVector_MPIPlusX**(*N_Vector* v)

> This function returns the local vector underneath the MPIPlusX NVECTOR.

sunindextype **N_VGetLocalLength_MPIPlusX**(*N_Vector* v)

> This function returns the local length of the vector underneath the MPIPlusX NVECTOR.
>
> Usage:

```
local_length = N_VGetLocalLength_MPIPlusX(v);
```

realtype ***N_VGetArrayPointer_MPIPlusX**(*N_Vector* v)

> This function returns the data array pointer for the local vector.

> If the local vector does not support the *N_VGetArrayPointer()* operation, then NULL is returned.

void **N_VSetArrayPointer_MPIPlusX**(*realtype* *v_data, *N_Vector* v)

> This function sets the data array pointer for the local vector if the local vector implements the *N_VSetArray-Pointer()* operation.

The NVECTOR_MPIPLUSX module does not implement any fused or vector array operations. Instead users should enable/disable fused operations on the local vector.

Notes

- *N_VMake_MPIPlusX()* sets the field own_data = SUNFALSE and N_VDestroy_MPIPlusX() will not call *N_-VDestroy()* on the local vector. In this a case, it is the user's responsibility to deallocate the local vector.

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

6.20 NVECTOR Examples

There are NVECTOR examples that may be installed for eac himplementation. Each implementation makes use of the functions in test_nvector.c. These example functions show simple usage of the NVECTOR family of functions. The input to the examples are the vector length, number of threads (if threaded implementation), and a print timing flag.

The following is a list of the example functions in test_nvector.c:

- Test_N_VClone: Creates clone of vector and checks validity of clone.

- Test_N_VCloneEmpty: Creates clone of empty vector and checks validity of clone.

- Test_N_VCloneVectorArray: Creates clone of vector array and checks validity of cloned array.

- Test_N_VCloneVectorArray: Creates clone of empty vector array and checks validity of cloned array.

- Test_N_VGetArrayPointer: Get array pointer.

- Test_N_VSetArrayPointer: Allocate new vector, set pointer to new vector array, and check values.

- Test_N_VGetLength: Compares self-reported length to calculated length.

- Test_N_VGetCommunicator: Compares self-reported communicator to the one used in constructor; or for MPI-unaware vectors it ensures that NULL is reported.

- Test_N_VLinearSum Case 1a: Test y = x + y

- Test_N_VLinearSum Case 1b: Test y = -x + y

- Test_N_VLinearSum Case 1c: Test y = ax + y

- Test_N_VLinearSum Case 2a: Test x = x + y

- Test_N_VLinearSum Case 2b: Test x = x - y

- Test_N_VLinearSum Case 2c: Test x = x + by

- `Test_N_VLinearSum` Case 3: Test z = x + y

- `Test_N_VLinearSum` Case 4a: Test z = x - y

- `Test_N_VLinearSum` Case 4b: Test z = -x + y

- `Test_N_VLinearSum` Case 5a: Test z = x + by

- `Test_N_VLinearSum` Case 5b: Test z = ax + y

- `Test_N_VLinearSum` Case 6a: Test z = -x + by

- `Test_N_VLinearSum` Case 6b: Test z = ax - y

- `Test_N_VLinearSum` Case 7: Test z = a(x + y)

- `Test_N_VLinearSum` Case 8: Test z = a(x - y)

- `Test_N_VLinearSum` Case 9: Test z = ax + by

- `Test_N_VConst`: Fill vector with constant and check result.

- `Test_N_VProd`: Test vector multiply: z = x * y

- `Test_N_VDiv`: Test vector division: z = x / y

- `Test_N_VScale`: Case 1: scale: x = cx

- `Test_N_VScale`: Case 2: copy: z = x

- `Test_N_VScale`: Case 3: negate: z = -x

- `Test_N_VScale`: Case 4: combination: z = cx

- `Test_N_VAbs`: Create absolute value of vector.

- `Test_N_VInv`: Compute z[i] = 1 / x[i]

** `Test_N_VAddConst`: add constant vector: z = c + x

- `Test_N_VDotProd`: Calculate dot product of two vectors.

- `Test_N_VMaxNorm`: Create vector with known values, find and validate the max norm.

- `Test_N_VWrmsNorm`: Create vector of known values, find and validate the weighted root mean square.

- `Test_N_VWrmsNormMask`: Create vector of known values, find and validate the weighted root mean square using all elements except one.

- `Test_N_VMin`: Create vector, find and validate the min.

- `Test_N_VWL2Norm`: Create vector, find and validate the weighted Euclidean L2 norm.

- `Test_N_VL1Norm`: Create vector, find and validate the L1 norm.

- `Test_N_VCompare`: Compare vector with constant returning and validating comparison vector.

- `Test_N_VInvTest`: Test z[i] = 1 / x[i]

- `Test_N_VConstrMask`: Test mask of vector x with vector c.

- `Test_N_VMinQuotient`: Fill two vectors with known values. Calculate and validate minimum quotient.

- `Test_N_VLinearCombination`: Case 1a: Test x = a x

- `Test_N_VLinearCombination`: Case 1b: Test z = a x

- `Test_N_VLinearCombination`: Case 2a: Test x = a x + b y

- `Test_N_VLinearCombination`: Case 2b: Test z = a x + b y

- `Test_N_VLinearCombination`: Case 3a: Test x = x + a y + b z

- `Test_N_VLinearCombination`: Case 3b: Test x = a x + b y + c z

- `Test_N_VLinearCombination`: Case 3c: Test w = a x + b y + c z

- `Test_N_VScaleAddMulti`: Case 1a: y = a x + y

- `Test_N_VScaleAddMulti`: Case 1b: z = a x + y

- `Test_N_VScaleAddMulti`: Case 2a: Y[i] = c[i] x + Y[i], i = 1,2,3

- `Test_N_VScaleAddMulti`: Case 2b: Z[i] = c[i] x + Y[i], i = 1,2,3

- `Test_N_VDotProdMulti`: Case 1: Calculate the dot product of two vectors

- `Test_N_VDotProdMulti`: Case 2: Calculate the dot product of one vector with three other vectors in a vector array.

- `Test_N_VLinearSumVectorArray`: Case 1: z = a x + b y

- `Test_N_VLinearSumVectorArray`: Case 2a: Z[i] = a X[i] + b Y[i]

- `Test_N_VLinearSumVectorArray`: Case 2b: X[i] = a X[i] + b Y[i]

- `Test_N_VLinearSumVectorArray`: Case 2c: Y[i] = a X[i] + b Y[i]

- `Test_N_VScaleVectorArray`: Case 1a: y = c y

- `Test_N_VScaleVectorArray`: Case 1b: z = c y

- `Test_N_VScaleVectorArray`: Case 2a: Y[i] = c[i] Y[i]

- `Test_N_VScaleVectorArray`: Case 2b: Z[i] = c[i] Y[i]

- `Test_N_VConstVectorArray`: Case 1a: z = c

- `Test_N_VConstVectorArray`: Case 1b: Z[i] = c

- `Test_N_VWrmsNormVectorArray`: Case 1a: Create a vector of know values, find and validate the weighted root mean square norm.

- `Test_N_VWrmsNormVectorArray`: Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each.

- `Test_N_VWrmsNormMaskVectorArray`: Case 1a: Create a vector of know values, find and validate the weighted root mean square norm using all elements except one.

- `Test_N_VWrmsNormMaskVectorArray`: Case 1b: Create a vector array of three vectors of know values, find and validate the weighted root mean square norm of each using all elements except one.

- `Test_N_VScaleAddMultiVectorArray`: Case 1a: y = a x + y

- `Test_N_VScaleAddMultiVectorArray`: Case 1b: z = a x + y

- `Test_N_VScaleAddMultiVectorArray`: Case 2a: Y[j][0] = a[j] X[0] + Y[j][0]

- `Test_N_VScaleAddMultiVectorArray`: Case 2b: Z[j][0] = a[j] X[0] + Y[j][0]

- `Test_N_VScaleAddMultiVectorArray`: Case 3a: Y[0][i] = a[0] X[i] + Y[0][i]

- `Test_N_VScaleAddMultiVectorArray`: Case 3b: Z[0][i] = a[0] X[i] + Y[0][i]

- `Test_N_VScaleAddMultiVectorArray`: Case 4a: Y[j][i] = a[j] X[i] + Y[j][i]

- `Test_N_VScaleAddMultiVectorArray`: Case 4b: Z[j][i] = a[j] X[i] + Y[j][i]

- `Test_N_VLinearCombinationVectorArray`: Case 1a: x = a x

- `Test_N_VLinearCombinationVectorArray`: Case 1b: z = a x

- `Test_N_VLinearCombinationVectorArray`: Case 2a: x = a x + b y

- `Test_N_VLinearCombinationVectorArray`: Case 2b: z = a x + b y

- `Test_N_VLinearCombinationVectorArray`: Case 3a: x = a x + b y + c z

- `Test_N_VLinearCombinationVectorArray`: Case 3b: w = a x + b y + c z

- `Test_N_VLinearCombinationVectorArray`: Case 4a: X[0][i] = c[0] X[0][i]

- `Test_N_VLinearCombinationVectorArray`: Case 4b: Z[i] = c[0] X[0][i]

- `Test_N_VLinearCombinationVectorArray`: Case 5a: X[0][i] = c[0] X[0][i] + c[1] X[1][i]

- `Test_N_VLinearCombinationVectorArray`: Case 5b: Z[i] = c[0] X[0][i] + c[1] X[1][i]

- `Test_N_VLinearCombinationVectorArray`: Case 6a: X[0][i] = X[0][i] + c[1] X[1][i] + c[2] X[2][i]

- `Test_N_VLinearCombinationVectorArray`: Case 6b: X[0][i] = c[0] X[0][i] + c[1] X[1][i] + c[2] X[2][i]

- `Test_N_VLinearCombinationVectorArray`: Case 6c: Z[i] = c[0] X[0][i] + c[1] X[1][i] + c[2] X[2][i]

- `Test_N_VDotProdLocal`: Calculate MPI task-local portion of the dot product of two vectors.

- `Test_N_VMaxNormLocal`: Create vector with known values, find and validate the MPI task-local portion of the max norm.

- `Test_N_VMinLocal`: Create vector, find and validate the MPI task-local min.

- `Test_N_VL1NormLocal`: Create vector, find and validate the MPI task-local portion of the L1 norm.

- `Test_N_VWSqrSumLocal`: Create vector of known values, find and validate the MPI task-local portion of the weighted squared sum of two vectors.

- `Test_N_VWSqrSumMaskLocal`: Create vector of known values, find and validate the MPI task-local portion of the weighted squared sum of two vectors, using all elements except one.

- `Test_N_VInvTestLocal`: Test the MPI task-local portion of z[i] = 1 / x[i]

- `Test_N_VConstrMaskLocal`: Test the MPI task-local portion of the mask of vector x with vector c.

- `Test_N_VMinQuotientLocal`: Fill two vectors with known values. Calculate and validate the MPI task-local minimum quotient.

- `Test_N_VMBufSize`: Tests for accuracy in the reported buffer size.

- `Test_N_VMBufPack`: Tests for accuracy in the buffer packing routine.

- `Test_N_VMBufUnpack`: Tests for accuracy in the buffer unpacking routine.

Chapter 7

Matrix Data Structures

The SUNDIALS library comes packaged with a variety of *SUNMatrix* implementations, designed for simulations requiring direct linear solvers for problems in serial or shared-memory parallel environments. SUNDIALS additionally provides a simple interface for generic matrices (akin to a C++ *abstract base class*). All of the major SUNDIALS packages (CVODE(s), IDA(s), KINSOL, ARKODE), are constructed to only depend on these generic matrix operations, making them immediately extensible to new user-defined matrix objects. For each of the SUNDIALS-provided matrix types, SUNDIALS also provides *SUNLinearSolver* implementations that factor these matrix objects and use them in the solution of linear systems.

7.1 Description of the SUNMATRIX Modules

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

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

typedef struct _generic_SUNMatrix ***SUNMatrix**

and the generic structure is defined as

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

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

```
struct _generic_SUNMatrix_Ops {
  SUNMatrix_ID (*getid)(SUNMatrix);
  SUNMatrix    (*clone)(SUNMatrix);
```

(continues on next page)

```
  void        (*destroy)(SUNMatrix);
  int         (*zero)(SUNMatrix);
  int         (*copy)(SUNMatrix, SUNMatrix);
  int         (*scaleadd)(realtype, SUNMatrix, SUNMatrix);
  int         (*scaleaddi)(realtype, SUNMatrix);
  int         (*matvecsetup)(SUNMatrix);
  int         (*matvec)(SUNMatrix, N_Vector, N_Vector);
  int         (*space)(SUNMatrix, long int*, long int*);
};
```

The generic SUNMATRIX module defines and implements the matrix operations acting on a `SUNMatrix`. These routines are nothing but wrappers for the matrix operations defined by a particular SUNMATRIX implementation, which are accessed through the *ops* field of the `SUNMatrix` structure. To illustrate this point we show below the implementation of a typical matrix operation from the generic SUNMATRIX module, namely `SUNMatZero`, which sets all values of a matrix `A` to zero, returning a flag denoting a successful/failed operation:

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

§7.2 contains a complete list of all matrix operations defined by the generic SUNMATRIX module. A particular implementation of the SUNMATRIX module must:

- Specify the *content* field of the `SUNMatrix` object.

- Define and implement a minimal subset of the matrix operations. See the documentation for each SUNDIALS package and/or linear solver to determine which SUNMATRIX operations they require.

  Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNMATRIX module (each with different `SUNMatrix` internal data representations) in the same code.

- Define and implement user-callable constructor and destructor routines to create and free a `SUNMatrix` with the new *content* field and with *ops* pointing to the new matrix operations.

- Optionally, define and implement additional user-callable routines acting on the newly defined `SUNMatrix` (e.g., a routine to print the *content* for debugging purposes).

- Optionally, provide accessor macros as needed for that particular implementation to be used to access different parts in the content field of the newly defined `SUNMatrix`.

To aid in the creation of custom SUNMATRIX modules the generic SUNMATRIX module provides three utility functions *SUNMatNewEmpty()*, *SUNMatCopyOps()*, and *SUNMatFreeEmpty()*. When used in custom SUNMATRIX constructors and clone routines these functions will ease the introduction of any new optional matrix operations to the SUNMATRIX API by ensuring only required operations need to be set and all operations are copied when cloning a matrix.

SUNMatrix **SUNMatNewEmpty**()

> This function allocates a new generic `SUNMatrix` object and initializes its content pointer and the function pointers in the operations structure to `NULL`.

> **Return value:**
>> If successful, this function returns a `SUNMatrix` object. If an error occurs when allocating the object, then this routine will return `NULL`.

int **SUNMatCopyOps**(*SUNMatrix* A, *SUNMatrix* B)

> This function copies the function pointers in the `ops` structure of `A` into the `ops` structure of `B`.

Arguments:

- *A* – the matrix to copy operations from.

- *B* – the matrix to copy operations to.

Return value:

If successful, this function returns `0`. If either of the inputs are `NULL` or the `ops` structure of either input is `NULL`, then is function returns a non-zero value.

void **SUNMatFreeEmpty**(*SUNMatrix* A)

This routine frees the generic `SUNMatrix` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.

Arguments:

- *A* – the SUNMatrix object to free

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

Table 7.1: Identifiers associated with matrix kernels supplied with SUN-DIALS

Matrix ID	Matrix type
SUNMATRIX_BAND	Band $M \times M$ matrix
SUNMATRIX_CUSPARSE	CUDA sparse CSR matrix
SUNMATRIX_CUSTOM	User-provided custom matrix
SUNMATRIX_DENSE	Dense $M \times N$ matrix
SUNMATRIX_GINKGO	SUNMatrix wraper for Ginkgo matrices
SUNMATRIX_MAGMADENSE	Dense $M \times N$ matrix
SUNMATRIX_ONEMKLDENSE	oneMKL dense $M \times N$ matrix
SUNMATRIX_SLUNRLOC	SUNMatrix wrapper for SuperLU_DIST SuperMatrix
SUNMATRIX_SPARSE	Sparse (CSR or CSC) $M \times N$ matrix

7.2 Description of the SUNMATRIX operations

For each of the `SUNMatrix` operations, we give the name, usage of the function, and a description of its mathematical operations below.

SUNMatrix_ID **SUNMatGetID**(*SUNMatrix* A)

Returns the type identifier for the matrix *A*. It is used to determine the matrix implementation type (e.g. dense, banded, sparse,...) from the abstract `SUNMatrix` interface. This is used to assess compatibility with SUNDIALS-provided linear solver implementations. Returned values are given in Table 7.1

Usage:

```
id = SUNMatGetID(A);
```

SUNMatrix **SUNMatClone**(*SUNMatrix* A)

Creates a new `SUNMatrix` of the same type as an existing matrix *A* and sets the *ops* field. It does not copy the matrix values, but rather allocates storage for the new matrix.

Usage:

```
B = SUNMatClone(A);
```

void **SUNMatDestroy**(*SUNMatrix* A)

    Destroys the SUNMatrix *A* and frees memory allocated for its internal data.

    Usage:

```
SUNMatDestroy(A);
```

int **SUNMatSpace**(*SUNMatrix* A, long int *lrw, long int *liw)

    Returns the storage requirements for the matrix *A*. *lrw* contains the number of realtype words and *liw* contains the number of integer words. The return value denotes success/failure of the operation.

    This function is advisory only, for use in determining a user's total space requirements; it could be a dummy function in a user-supplied SUNMatrix module if that information is not of interest.

    Usage:

```
retval = SUNMatSpace(A, &lrw, &liw);
```

int **SUNMatZero**(*SUNMatrix* A)

    Zeros all entries of the SUNMatrix *A*. The return value is an integer flag denoting success/failure of the operation:

$$A_{i,j} = 0, \quad i = 1, \ldots, m, \; j = 1, \ldots, n.$$

    Usage:

```
retval = SUNMatZero(A);
```

int **SUNMatCopy**(*SUNMatrix* A, *SUNMatrix* B)

    Performs the operation *B gets A* for all entries of the matrices *A* and *B*. The return value is an integer flag denoting success/failure of the operation:

$$B_{i,j} = A_{i,j}, \quad i = 1, \ldots, m, \; j = 1, \ldots, n.$$

    Usage:

```
retval = SUNMatCopy(A,B);
```

int **SUNMatScaleAdd**(*realtype* c, *SUNMatrix* A, *SUNMatrix* B)

    Performs the operation *A gets cA + B*. The return value is an integer flag denoting success/failure of the operation:

$$A_{i,j} = cA_{i,j} + B_{i,j}, \quad i = 1, \ldots, m, \; j = 1, \ldots, n.$$

    Usage:

```
retval = SUNMatScaleAdd(c, A, B);
```

int **SUNMatScaleAddI**(*realtype* c, *SUNMatrix* A)

    Performs the operation *A gets cA + I*. The return value is an integer flag denoting success/failure of the operation:

$$A_{i,j} = cA_{i,j} + \delta_{i,j}, \quad i, j = 1, \ldots, n.$$

    Usage:

```
retval = SUNMatScaleAddI(c, A);
```

int **SUNMatMatvecSetup**(*SUNMatrix* A)

Performs any setup necessary to perform a matrix-vector product. The return value is an integer flag denoting success/failure of the operation. It is useful for SUNMatrix implementations which need to prepare the matrix itself, or communication structures before performing the matrix-vector product.

Usage:

```
retval = SUNMatMatvecSetup(A);
```

int **SUNMatMatvec**(*SUNMatrix* A, *N_Vector* x, *N_Vector* y)

Performs the matrix-vector product *y gets Ax*. It should only be called with vectors *x* and *y* that are compatible with the matrix *A* – both in storage type and dimensions. The return value is an integer flag denoting success/failure of the operation:

$$y_i = \sum_{j=1}^{n} A_{i,j} x_j, \quad i = 1, \ldots, m.$$

Usage:

```
retval = SUNMatMatvec(A, x, y);
```

7.2.1 SUNMatrix return codes

The functions provided to SUNMatrix modules within the SUNDIALS-provided SUNMatrix implementations utilize a common set of return codes, listed below. These adhere to a common pattern: 0 indicates success, a negative value indicates a failure. Aside from this pattern, the actual values of each error code are primarily to provide additional information to the user in case of a SUNMatrix failure.

- `SUNMAT_SUCCESS` (0) – successful call
- `SUNMAT_ILL_INPUT` (-1) – an illegal input has been provided to the function
- `SUNMAT_MEM_FAIL` (-2) – failed memory access or allocation
- `SUNMAT_OPERATION_FAIL` (-3) – a SUNMatrix operation returned nonzero
- `SUNMAT_MATVEC_SETUP_REQUIRED` (-4) – the *SUNMatMatvecSetup()* routine needs to be called prior to calling *SUNMatMatvec()*

7.3 The SUNMATRIX_DENSE Module

The dense implementation of the `SUNMatrix` module, SUNMATRIX_DENSE, defines the *content* field of `SUNMatrix` to be the following structure:

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

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

- `M` - number of rows

- `N` - number of columns

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

- `ldata` - length of the data array ($= M\,N$).

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

The header file to be included when using this module is `sunmatrix/sunmatrix_dense.h`.

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

SM_CONTENT_D(A)

> This macro gives access to the contents of the dense `SUNMatrix` A.

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

> Implementation:

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

SM_ROWS_D(A)

> Access the number of rows in the dense `SUNMatrix` A.

> This may be used either to retrieve or to set the value. For example, the assignment `A_rows = SM_ROWS_D(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_ROWS_D(A) = A_rows` sets the number of columns in `A` to equal `A_rows`.

> Implementation:

> ```
> #define SM_ROWS_D(A)   ( SM_CONTENT_D(A)->M )
> ```

SM_COLUMNS_D(A)

> Access the number of columns in the dense `SUNMatrix` A.

> This may be used either to retrieve or to set the value. For example, the assignment `A_columns = SM_-COLUMNS_D(A)` sets `A_columns` to be the number of columns in the matrix `A`. Similarly, the assignment `SM_-COLUMNS_D(A) = A_columns` sets the number of columns in `A` to equal `A_columns`

> Implementation:

> ```
> #define SM_COLUMNS_D(A)   ( SM_CONTENT_D(A)->N )
> ```

SM_LDATA_D(A)

> Access the total data length in the dense `SUNMatrix` A.

> This may be used either to retrieve or to set the value. For example, the assignment `A_ldata = SM_LDATA_-D(A)` sets `A_ldata` to be the length of the data array in the matrix `A`. Similarly, the assignment `SM_LDATA_D(A) = A_ldata` sets the parameter for the length of the data array in `A` to equal `A_ldata`.

> Implementation:

```
#define SM_LDATA_D(A)    ( SM_CONTENT_D(A)->ldata )
```

SM_DATA_D(A)

This macro gives access to the `data` pointer for the matrix entries.

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

Implementation:

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

SM_COLS_D(A)

This macro gives access to the `cols` pointer for the matrix entries.

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

Implementation:

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

SM_COLUMN_D(A)

This macros gives access to the individual columns of the data array of a dense SUNMatrix.

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

Implementation:

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

SM_ELEMENT_D(A)

This macro gives access to the individual entries of the data array of a dense SUNMatrix.

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

Implementation:

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

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

SUNMatrix **SUNDenseMatrix**(*sunindextype* M, *sunindextype* N, *SUNContext* sunctx)

This constructor function creates and allocates memory for a dense SUNMatrix. Its arguments are the number of rows, M, and columns, N, for the dense matrix.

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

This function prints the content of a dense SUNMatrix to the output stream specified by `outfile`. Note: `std-out` or `stderr` may be used as arguments for `outfile` to print directly to standard output or standard error, respectively.

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sunindextype **SUNDenseMatrix_Rows**(*SUNMatrix* A)

   This function returns the number of rows in the dense SUNMatrix.

sunindextype **SUNDenseMatrix_Columns**(*SUNMatrix* A)

   This function returns the number of columns in the dense SUNMatrix.

sunindextype **SUNDenseMatrix_LData**(*SUNMatrix* A)

   This function returns the length of the data array for the dense SUNMatrix.

realtype ***SUNDenseMatrix_Data**(*SUNMatrix* A)

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

realtype ****SUNDenseMatrix_Cols**(*SUNMatrix* A)

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

realtype ***SUNDenseMatrix_Column**(*SUNMatrix* A, *sunindextype* j)

   This function returns a pointer to the first entry of the jth column of the dense SUNMatrix. The resulting pointer should be indexed over the range `0` to `M-1`.

Notes

- When looping over the components of a dense SUNMatrix `A`, the most efficient approaches are to:

  - First obtain the component array via `A_data = SUNDenseMatrix_Data(A)`, or equivalently `A_data = SM_DATA_D(A)`, and then access `A_data[i]` within the loop.

  - First obtain the array of column pointers via `A_cols = SUNDenseMatrix_Cols(A)`, or equivalently `A_cols = SM_COLS_D(A)`, and then access `A_cols[j][i]` within the loop.

  - Within a loop over the columns, access the column pointer via `A_colj = SUNDenseMatrix_Column(A, j)` and then to access the entries within that column using `A_colj[i]` within the loop.

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

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

7.4 The SUNMATRIX_MAGMADENSE Module

The SUNMATRIX_MAGMADENSE module interfaces to the MAGMA linear algebra library and can target NVIDIA's CUDA programming model or AMD's HIP programming model [53]. All data stored by this matrix implementation resides on the GPU at all times. The implementation currently supports a standard LAPACK column-major storage format as well as a low-storage format for block-diagonal matrices

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix}$$

This matrix implementation is best paired with the *SUNLinearSolver_MagmaDense* SUNLinearSolver.

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

Warning: The SUNMATRIX_MAGMADENSE module is experimental and subject to change.

7.4.1 SUNMATRIX_MAGMADENSE Functions

The SUNMATRIX_MAGMADENSE module defines GPU-enabled implementations of all matrix operations listed in §7.2.

- `SUNMatGetID_MagmaDense` – returns `SUNMATRIX_MAGMADENSE`
- `SUNMatClone_MagmaDense`
- `SUNMatDestroy_MagmaDense`
- `SUNMatZero_MagmaDense`
- `SUNMatCopy_MagmaDense`
- `SUNMatScaleAdd_MagmaDense`
- `SUNMatScaleAddI_MagmaDense`
- `SUNMatMatvecSetup_MagmaDense`
- `SUNMatMatvec_MagmaDense`
- `SUNMatSpace_MagmaDense`

In addition, the SUNMATRIX_MAGMADENSE module defines the following implementation specific functions:

SUNMatrix **SUNMatrix_MagmaDense**(*sunindextype* M, *sunindextype* N, *SUNMemoryType* memtype, *SUNMemoryHelper* memhelper, void *queue, *SUNContext* sunctx)

This constructor function creates and allocates memory for an $M \times N$ SUNMATRIX_MAGMADENSE SUN-Matrix.

Arguments:

- *M* – the number of matrix rows.
- *N* – the number of matrix columns.
- *memtype* – the type of memory to use for the matrix data; can be `SUNMEMTYPE_UVM` or `SUNMEMTYPE_-DEVICE`.
- *memhelper* – the memory helper used for allocating data.
- *queue* – a `cudaStream_t` when using CUDA or a `hipStream_t` when using HIP.
- *sunctx* – the *SUNContext* object (see §4.1)

Return value:
If successful, a SUNMatrix object otherwise NULL.

SUNMatrix **SUNMatrix_MagmaDenseBlock**(*sunindextype* nblocks, *sunindextype* M_block, *sunindextype* N_block, *SUNMemoryType* memtype, *SUNMemoryHelper* memhelper, void *queue, *SUNContext* sunctx)

This constructor function creates and allocates memory for a block diagonal SUNMATRIX_MAGMADENSE SUNMatrix with *nblocks* of size $M \times N$.

Arguments:

- *nblocks* – the number of matrix rows.
- *M_block* – the number of matrix rows in each block.

- *N_block* – the number of matrix columns in each block.

- *memtype* – the type of memory to use for the matrix data; can be SUNMEMTYPE_UVM or SUNMEMTYPE_-DEVICE.

- *memhelper* – the memory helper used for allocating data.

- *queue* – a cudaStream_t when using CUDA or a hipStream_t when using HIP.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

If successful, a SUNMatrix object otherwise NULL.

sunindextype **SUNMatrix_MagmaDense_Rows**(*SUNMatrix* A)

This function returns the number of rows in the SUNMatrix object. For block diagonal matrices, the number of rows is computed as $M_{\text{block}} \times$ nblocks.

Arguments:

- *A* – a SUNMatrix object.

Return value:

If successful, the number of rows in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_MagmaDense_Columns**(*SUNMatrix* A)

This function returns the number of columns in the SUNMatrix object. For block diagonal matrices, the number of columns is computed as $N_{\text{block}} \times$ nblocks.

Arguments:

- *A* – a SUNMatrix object.

Return value:

If successful, the number of columns in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_MagmaDense_BlockRows**(*SUNMatrix* A)

This function returns the number of rows in a block of the SUNMatrix object.

Arguments:

- *A* – a SUNMatrix object.

Return value:

If successful, the number of rows in a block of the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_MagmaDense_BlockColumns**(*SUNMatrix* A)

This function returns the number of columns in a block of the SUNMatrix object.

Arguments:

- *A* – a SUNMatrix object.

Return value:

If successful, the number of columns in a block of the SUNMatrix object otherwise SUNMATRIX_ILL_-INPUT.

sunindextype **SUNMatrix_MagmaDense_LData**(*SUNMatrix* A)

This function returns the length of the SUNMatrix data array.

Arguments:

- *A* – a SUNMatrix object.

Return value:
   If successful, the length of the SUNMatrix data array otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_MagmaDense_NumBlocks**(*SUNMatrix* A)
   This function returns the number of blocks in the SUNMatrix object.

   Arguments:

   - *A* – a SUNMatrix object.

   Return value:
      If successful, the number of blocks in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

realtype ***SUNMatrix_MagmaDense_Data**(*SUNMatrix* A)
   This function returns the SUNMatrix data array.

   Arguments:

   - *A* – a SUNMatrix object.

   Return value:
      If successful, the SUNMatrix data array otherwise NULL.

realtype ****SUNMatrix_MagmaDense_BlockData**(*SUNMatrix* A)
   This function returns an array of pointers that point to the start of the data array for each block in the SUNMatrix.

   Arguments:

   - *A* – a SUNMatrix object.

   Return value:
      If successful, an array of data pointers to each of the SUNMatrix blocks otherwise NULL.

realtype ***SUNMatrix_MagmaDense_Block**(*SUNMatrix* A, *sunindextype* k)
   This function returns a pointer to the data array for block k in the SUNMatrix.

   Arguments:

   - *A* – a SUNMatrix object.
   - *k* – the block index.

   Return value:
      If successful, a pointer to the data array for the SUNMatrix block otherwise NULL.

   Note: No bounds-checking is performed by this function, j should be strictly less than *nblocks*.

   ---

realtype ***SUNMatrix_MagmaDense_Column**(*SUNMatrix* A, *sunindextype* j)
   This function returns a pointer to the data array for column j in the SUNMatrix.

   Arguments:

   - *A* – a SUNMatrix object.
   - *j* – the column index.

   Return value:
      If successful, a pointer to the data array for the SUNMatrix column otherwise NULL.

   Note: No bounds-checking is performed by this function, j should be strictly less than $nblocks * N_{\text{block}}$.

   ---

realtype ***SUNMatrix_MagmaDense_BlockColumn**(*SUNMatrix* A, *sunindextype* k, *sunindextype* j)

    This function returns a pointer to the data array for column *j* of block *k* in the `SUNMatrix`.

    Arguments:

- *A* – a `SUNMatrix` object.
- *k* – the block index.
- *j* – the column index.

    Return value:

        If successful, a pointer to the data array for the `SUNMatrix` column otherwise `NULL`.

Note: No bounds-checking is performed by this function, *k* should be strictly less than *nblocks* and *j* should be strictly less than N_{block}.

---

int **SUNMatrix_MagmaDense_CopyToDevice**(*SUNMatrix* A, *realtype* *h_data)

    This function copies the matrix data to the GPU device from the provided host array.

    Arguments:

- *A* – a `SUNMatrix` object
- *h_data* – a host array pointer to copy data from.

    Return value:

- `SUNMAT_SUCCESS` – if the copy is successful.
- `SUNMAT_ILL_INPUT` – if either the `SUNMatrix` is not a `SUNMATRIX_MAGMADENSE` matrix.
- `SUNMAT_MEM_FAIL` – if the copy fails.

int **SUNMatrix_MagmaDense_CopyFromDevice**(*SUNMatrix* A, *realtype* *h_data)

    This function copies the matrix data from the GPU device to the provided host array.

    Arguments:

- *A* – a `SUNMatrix` object
- *h_data* – a host array pointer to copy data to.

    Return value:

- `SUNMAT_SUCCESS` – if the copy is successful.
- `SUNMAT_ILL_INPUT` – if either the `SUNMatrix` is not a `SUNMATRIX_MAGMADENSE` matrix.
- `SUNMAT_MEM_FAIL` – if the copy fails.

7.4.2 SUNMATRIX_MAGMADENSE Usage Notes

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

7.5 The SUNMATRIX_ONEMKLDENSE Module

The SUNMATRIX_ONEMKLDENSE module is intended for interfacing with direct linear solvers from the Intel oneAPI Math Kernel Library (oneMKL) using the SYCL (DPC++) programming model. The implementation currently supports a standard LAPACK column-major storage format as well as a low-storage format for block-diagonal matrices,

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix}$$

This matrix implementation is best paired with the *SUNLinearSolver_OneMklDense* linear solver.

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

> **Warning:** The SUNMATRIX_ONEMKLDENSE class is experimental and subject to change.

7.5.1 SUNMATRIX_ONEMKLDENSE Functions

The SUNMATRIX_ONEMKLDENSE class defines implementations of the following matrix operations listed in §7.2.

- `SUNMatGetID_OneMklDense` – returns `SUNMATRIX_ONEMKLDENSE`

- `SUNMatClone_OneMklDense`

- `SUNMatDestroy_OneMklDense`

- `SUNMatZero_OneMklDense`

- `SUNMatCopy_OneMklDense`

- `SUNMatScaleAdd_OneMklDense`

- `SUNMatScaleAddI_OneMklDense`

- `SUNMatMatvec_OneMklDense`

- `SUNMatSpace_OneMklDense`

In addition, the SUNMATRIX_ONEMKLDENSE class defines the following implementation specific functions.

7.5.1.1 Constructors

SUNMatrix **SUNMatrix_OneMklDense**(sunindextype M, sunindextype N, SUNMemoryType memtype,
                                          SUNMemoryHelper memhelper, sycl::queue *queue, SUNContext sunctx)

This constructor function creates and allocates memory for an $M \times N$ SUNMATRIX_ONEMKLDENSE SUN-Matrix.

Arguments:

- *M* – the number of matrix rows.

- *N* – the number of matrix columns.

- *memtype* – the type of memory to use for the matrix data; can be `SUNMEMTYPE_UVM` or `SUNMEMTYPE_-DEVICE`.

- *memhelper* – the memory helper used for allocating data.

- *queue* – the SYCL queue to which operations will be submitted.

- *sunctx* – the [*SUNContext*](#) object (see §4.1)

Return value:
If successful, a SUNMatrix object otherwise NULL.

SUNMatrix **SUNMatrix_OneMklDenseBlock**(sunindextype nblocks, sunindextype M_block, sunindextype N_block, SUNMemoryType memtype, SUNMemoryHelper memhelper, sycl::queue *queue, SUNContext sunctx)

This constructor function creates and allocates memory for a block diagonal SUNMATRIX_ONEMKLDENSE SUNMatrix with *nblocks* of size $M_{block} \times N_{block}$.

Arguments:

- *nblocks* – the number of matrix rows.

- *M_block* – the number of matrix rows in each block.

- *N_block* – the number of matrix columns in each block.

- *memtype* – the type of memory to use for the matrix data; can be SUNMEMTYPE_UVM or SUNMEMTYPE_-DEVICE.

- *memhelper* – the memory helper used for allocating data.

- *queue* – the SYCL queue to which operations will be submitted.

- *sunctx* – the [*SUNContext*](#) object (see §4.1)

Return value:
If successful, a SUNMatrix object otherwise NULL.

7.5.1.2 Access Matrix Dimensions

sunindextype **SUNMatrix_OneMklDense_Rows**(*SUNMatrix* A)

This function returns the number of rows in the SUNMatrix object. For block diagonal matrices, the number of rows is computed as $M_{block} \times$ nblocks.

Arguments:

- *A* – a SUNMatrix object.

Return value:
If successful, the number of rows in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_OneMklDense_Columns**(*SUNMatrix* A)

This function returns the number of columns in the SUNMatrix object. For block diagonal matrices, the number of columns is computed as $N_{block} \times$ nblocks.

Arguments:

- *A* – a SUNMatrix object.

Return value:
If successful, the number of columns in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

7.5.1.3 Access Matrix Block Dimensions

sunindextype **SUNMatrix_OneMklDense_NumBlocks**(*SUNMatrix* A)

 This function returns the number of blocks in the SUNMatrix object.

 Arguments:

   • *A* – a SUNMatrix object.

 Return value:

  If successful, the number of blocks in the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_OneMklDense_BlockRows**(*SUNMatrix* A)

 This function returns the number of rows in a block of the SUNMatrix object.

 Arguments:

   • *A* – a SUNMatrix object.

 Return value:

  If successful, the number of rows in a block of the SUNMatrix object otherwise SUNMATRIX_ILL_INPUT.

sunindextype **SUNMatrix_OneMklDense_BlockColumns**(*SUNMatrix* A)

 This function returns the number of columns in a block of the SUNMatrix object.

 Arguments:

   • *A* – a SUNMatrix object.

 Return value:

  If successful, the number of columns in a block of the SUNMatrix object otherwise SUNMATRIX_ILL_-
  INPUT.

7.5.1.4 Access Matrix Data

sunindextype **SUNMatrix_OneMklDense_LData**(*SUNMatrix* A)

 This function returns the length of the SUNMatrix data array.

 Arguments:

   • *A* – a SUNMatrix object.

 Return value:

  If successful, the length of the SUNMatrix data array otherwise SUNMATRIX_ILL_INPUT.

realtype ***SUNMatrix_OneMklDense_Data**(*SUNMatrix* A)

 This function returns the SUNMatrix data array.

 Arguments:

   • *A* – a SUNMatrix object.

 Return value:

  If successful, the SUNMatrix data array otherwise NULL.

realtype ***SUNMatrix_OneMklDense_Column**(*SUNMatrix* A, *sunindextype* j)

 This function returns a pointer to the data array for column j in the SUNMatrix.

 Arguments:

   • *A* – a SUNMatrix object.

   • *j* – the column index.

Return value:
> If successful, a pointer to the data array for the SUNMatrix column otherwise NULL.

Note: No bounds-checking is performed by this function, j should be strictly less than $nblocks * N_{\text{block}}$.

7.5.1.5 Access Matrix Block Data

sunindextype **SUNMatrix_OneMklDense_BlockLData**(*SUNMatrix* A)

> This function returns the length of the SUNMatrix data array for each block of the SUNMatrix object.

> **Arguments:**
>> • *A* – a SUNMatrix object.

> **Return value:**
>> If successful, the length of the SUNMatrix data array for each block otherwise SUNMATRIX_ILL_INPUT.

realtype ****SUNMatrix_OneMklDense_BlockData**(*SUNMatrix* A)

> This function returns an array of pointers that point to the start of the data array for each block in the SUNMatrix.

> **Arguments:**
>> • *A* – a SUNMatrix object.

> **Return value:**
>> If successful, an array of data pointers to each of the SUNMatrix blocks otherwise NULL.

realtype ***SUNMatrix_OneMklDense_Block**(*SUNMatrix* A, *sunindextype* k)

> This function returns a pointer to the data array for block k in the SUNMatrix.

> **Arguments:**
>> • *A* – a SUNMatrix object.
>>
>> • *k* – the block index.

> **Return value:**
>> If successful, a pointer to the data array for the SUNMatrix block otherwise NULL.

Note: No bounds-checking is performed by this function, j should be strictly less than *nblocks*.

---

realtype ***SUNMatrix_OneMklDense_BlockColumn**(*SUNMatrix* A, *sunindextype* k, *sunindextype* j)

> This function returns a pointer to the data array for column j of block k in the SUNMatrix.

> **Arguments:**
>> • *A* – a SUNMatrix object.
>>
>> • *k* – the block index.
>>
>> • *j* – the column index.

> **Return value:**
>> If successful, a pointer to the data array for the SUNMatrix column otherwise NULL.

Note: No bounds-checking is performed by this function, k should be strictly less than *nblocks* and j should be strictly less than N_{block}.

7.5.1.6 Copy Data

int **SUNMatrix_OneMklDense_CopyToDevice**(*SUNMatrix* A, *realtype* *h_data)

> This function copies the matrix data to the GPU device from the provided host array.
>
> **Arguments:**
>
> - *A* – a SUNMatrix object
> - *h_data* – a host array pointer to copy data from.
>
> **Return value:**
>
> - SUNMAT_SUCCESS – if the copy is successful.
> - SUNMAT_ILL_INPUT – if either the SUNMatrix is not a SUNMATRIX_ONEMKLDENSE matrix.
> - SUNMAT_MEM_FAIL – if the copy fails.

int **SUNMatrix_OneMklDense_CopyFromDevice**(*SUNMatrix* A, *realtype* *h_data)

> This function copies the matrix data from the GPU device to the provided host array.
>
> **Arguments:**
>
> - *A* – a SUNMatrix object
> - *h_data* – a host array pointer to copy data to.
>
> **Return value:**
>
> - SUNMAT_SUCCESS – if the copy is successful.
> - SUNMAT_ILL_INPUT – if either the SUNMatrix is not a SUNMATRIX_ONEMKLDENSE matrix.
> - SUNMAT_MEM_FAIL – if the copy fails.

7.5.2 SUNMATRIX_ONEMKLDENSE Usage Notes

> **Warning:** The SUNMATRIX_ONEMKLDENSE class only supports 64-bit indexing, thus SUNDIALS must be built for 64-bit indexing to use this class.
>
> When using the SUNMATRIX_ONEMKLDENSE class with a SUNDIALS package (e.g. CVODE), the queue given to matrix should be the same stream used for the NVECTOR object that is provided to the package, and the NVECTOR object given to the *SUNMatMatvec()* operation. If different streams are utilized, synchronization issues may occur.

7.6 The SUNMATRIX_BAND Module

The banded implementation of the SUNMatrix module, SUNMATRIX_BAND, defines the *content* field of SUNMatrix to be the following structure:

```
struct _SUNMatrixContent_Band {
  sunindextype M;
  sunindextype N;
  sunindextype mu;
  sunindextype ml;
  sunindextype smu;
```

```
  sunindextype ldim;
  realtype *data;
  sunindextype ldata;
  realtype **cols;
};
```

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

- `M` - number of rows

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

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

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

- `smu` - storage upper bandwidth, $\text{mu} \leq \text{smu} < N$. The LU decomposition routines in the associated *SUN-LINSOL_BAND* and *SUNLINSOL_LAPACKBAND* modules write the LU factors into the existing storage for the band matrix. The upper triangular factor U, however, may have an upper bandwidth as big as `min(N-1, mu+ml)` because of partial pivoting. The `smu` field holds the upper half-bandwidth allocated for the band matrix.

- `ldim` - leading dimension (ldim $\geq smu + ml + 1$)

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

- `ldata` - length of the data array ($= \text{ldim} \, N$)

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

The header file to be included when using this module is `sunmatrix/sunmatrix_band.h`.

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

`SM_CONTENT_B`(A)

This macro gives access to the contents of the banded `SUNMatrix` A.

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

Implementation:

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

`SM_ROWS_B`(A)

Access the number of rows in the banded `SUNMatrix` A.

This may be used either to retrieve or to set the value. For example, the assignment `A_rows = SM_ROWS_B(A)` sets `A_rows` to be the number of rows in the matrix `A`. Similarly, the assignment `SM_ROWS_B(A) = A_rows` sets the number of columns in `A` to equal `A_rows`.

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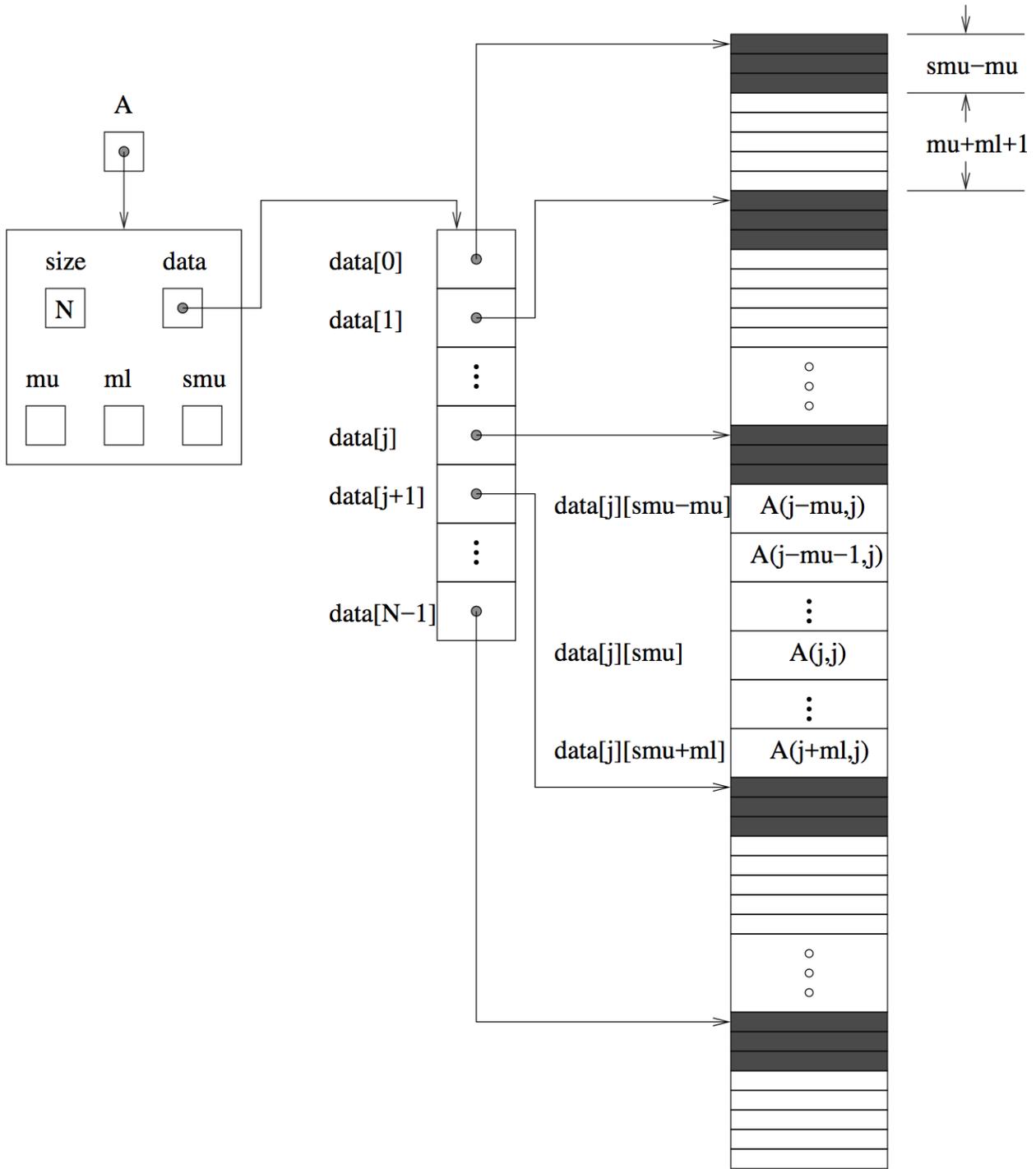
Fig. 7.1: Diagram of the storage for the SUNMATRIX_BAND module. Here A is an $N \times N$ band matrix with upper and lower half-bandwidths mu and ml, respectively. The rows and columns of A are numbered from 0 to N-1 and the (i, j)-th element of A is denoted A(i,j). The greyed out areas of the underlying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

```
#define SM_ROWS_B(A)    ( SM_CONTENT_B(A)->M )
```

SM_COLUMNS_B(A)

Access the number of columns in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_COLUMNS_B(A)    ( SM_CONTENT_B(A)->N )
```

SM_UBAND_B(A)

Access the mu parameter in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_UBAND_B(A)    ( SM_CONTENT_B(A)->mu )
```

SM_LBAND_B(A)

Access the ml parameter in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_LBAND_B(A)    ( SM_CONTENT_B(A)->ml )
```

SM_SUBAND_B(A)

Access the smu parameter in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_SUBAND_B(A)    ( SM_CONTENT_B(A)->smu )
```

SM_LDIM_B(A)

Access the ldim parameter in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_LDIM_B(A)    ( SM_CONTENT_B(A)->ldim )
```

SM_LDATA_B(A)

Access the ldata parameter in the banded SUNMatrix *A*. As with SM_ROWS_B, this may be used either to retrieve or to set the value.

Implementation:

```
#define SM_LDATA_B(A)    ( SM_CONTENT_B(A)->ldata )
```

SM_DATA_B(A)

This macro gives access to the data pointer for the matrix entries.

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

Implementation:

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

SM_COLS_B(A)

This macro gives access to the `cols` pointer for the matrix entries.

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

Implementation:

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

SM_COLUMN_B(A)

This macros gives access to the individual columns of the data array of a banded `SUNMatrix`.

The assignment `col_j = SM_COLUMN_B(A,j)` sets `col_j` to be a pointer to the diagonal element of the j-th column of the $N \times N$ band matrix `A`, $0 \leq j \leq N - 1$. The type of the expression `SM_COLUMN_B(A,j)` is `realtype *`. The pointer returned by the call `SM_COLUMN_B(A,j)` can be treated as an array which is indexed from `-mu` to `ml`.

Implementation:

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

SM_ELEMENT_B(A)

This macro gives access to the individual entries of the data array of a banded `SUNMatrix`.

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

Implementation:

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

SM_COLUMN_ELEMENT_B(A)

This macro gives access to the individual entries of the data array of a banded `SUNMatrix`.

The assignments `SM_COLUMN_ELEMENT_B(col_j,i,j) = a_ij` and `a_ij = SM_COLUMN_ELEMENT_-B(col_j,i,j)` reference the (i, j)-th entry of the band matrix `A` when used in conjunction with `SM_COLUMN_B` to reference the j-th column through `col_j`. The index (i, j) should satisfy $j - \mathrm{mu} \leq i \leq j + \mathrm{ml}$.

Implementation:

```
#define SM_COLUMN_ELEMENT_B(col_j,i,j)    (col_j[(i)-(j)])
```

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

SUNMatrix **SUNBandMatrix**(*sunindextype* N, *sunindextype* mu, *sunindextype* ml, *SUNContext* sunctx)

This constructor function creates and allocates memory for a banded `SUNMatrix`. Its arguments are the matrix size, `N`, and the upper and lower half-bandwidths of the matrix, `mu` and `ml`. The stored upper bandwidth is set to `mu+ml` to accommodate subsequent factorization in the SUNLINSOL_BAND and SUNLINSOL_LAPACK-BAND modules.

SUNMatrix **SUNBandMatrixStorage**(*sunindextype* N, *sunindextype* mu, *sunindextype* ml, *sunindextype* smu, *SUNContext* sunctx)

This constructor function creates and allocates memory for a banded SUNMatrix. Its arguments are the matrix size, N, the upper and lower half-bandwidths of the matrix, mu and ml, and the stored upper bandwidth, smu. When creating a band SUNMatrix, this value should be

- at least min(N-1,mu+ml) if the matrix will be used by the SUNLinSol_Band module;

- exactly equal to mu+ml if the matrix will be used by the SUNLinSol_LapackBand module;

- at least mu if used in some other manner.

Note: It is strongly recommended that users call the default constructor, *SUNBandMatrix()*, in all standard use cases. This advanced constructor is used internally within SUNDIALS solvers, and is provided to users who require banded matrices for non-default purposes.

---

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

This function prints the content of a banded SUNMatrix to the output stream specified by outfile. Note: stdout or stderr may be used as arguments for outfile to print directly to standard output or standard error, respectively.

sunindextype **SUNBandMatrix_Rows**(*SUNMatrix* A)

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

sunindextype **SUNBandMatrix_Columns**(*SUNMatrix* A)

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

sunindextype **SUNBandMatrix_LowerBandwidth**(*SUNMatrix* A)

This function returns the lower half-bandwidth for the banded SUNMatrix.

sunindextype **SUNBandMatrix_UpperBandwidth**(*SUNMatrix* A)

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

sunindextype **SUNBandMatrix_StoredUpperBandwidth**(*SUNMatrix* A)

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

sunindextype **SUNBandMatrix_LDim**(*SUNMatrix* A)

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

sunindextype **SUNBandMatrix_LData**(*SUNMatrix* A)

This function returns the length of the data array for the banded SUNMatrix.

realtype ***SUNBandMatrix_Data**(*SUNMatrix* A)

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

realtype ****SUNBandMatrix_Cols**(*SUNMatrix* A)

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

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

This function returns a pointer to the diagonal entry of the j-th column of the banded SUNMatrix. The resulting pointer should be indexed over the range -mu to ml.

Warning: When calling this function from the Fortran interfaces the shape of the array that is returned is [1], and the only element you can (legally) access is the diagonal element. Fortran users should instead work with the data array returned by *SUNBandMatrix_Data()* directly.

Notes

- When looping over the components of a banded SUNMatrix A, the most efficient approaches are to:

  - First obtain the component array via A_data = SUNBandMatrix_Data(A), or equivalently A_data = SM_DATA_B(A), and then access A_data[i] within the loop.

  - First obtain the array of column pointers via A_cols = SUNBandMatrix_Cols(A), or equivalently A_cols = SM_COLS_B(A), and then access A_cols[j][i] within the loop.

  - Within a loop over the columns, access the column pointer via A_colj = SUNBandMatrix_Column(A,j) and then to access the entries within that column using SM_COLUMN_ELEMENT_B(A_colj,i,j).

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

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

7.7 The SUNMATRIX_CUSPARSE Module

The SUNMATRIX_CUSPARSE module is an interface to the NVIDIA cuSPARSE matrix for use on NVIDIA GPUs [6]. All data stored by this matrix implementation resides on the GPU at all times.

The header file to be included when using this module is sunmatrix/sunmatrix_cusparse.h. The installed library to link to is libsundials_sunmatrixcusparse.lib where .lib is typically .so for shared libraries and .a for static libraries.

7.7.1 SUNMATRIX_CUSPARSE Description

The implementation currently supports the cuSPARSE CSR matrix format described in the cuSPARSE documentation, as well as a unique low-storage format for block-diagonal matrices of the form

$$
\mathbf{A} = \begin{bmatrix} \mathbf{A_0} & 0 & \cdots & 0 \\ 0 & \mathbf{A_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A_{n-1}} \end{bmatrix},
$$

where all the block matrices $\mathbf{A_j}$ share the same sparsity pattern. We will refer to this format as BCSR (not to be confused with the canonical BSR format where each block is stored as dense). In this format, the CSR column indices and row pointers are only stored for the first block and are computed only as necessary for other blocks. This can drastically reduce the amount of storage required compared to the regular CSR format when the number of blocks is large. This format is well-suited for, and intended to be used with, the SUNLinearSolver_cuSolverSp_batchQR linear solver (see §8.17).

The SUNMATRIX_CUSPARSE module is experimental and subject to change.

7.7.2 SUNMATRIX_CUSPARSE Functions

The SUNMATRIX_CUSPARSE module defines GPU-enabled sparse implementations of all matrix operations listed in §7.2 except for the *SUNMatSpace()* and *SUNMatMatvecSetup()* operations:

- `SUNMatGetID_cuSparse` – returns `SUNMATRIX_CUSPARSE`

- `SUNMatClone_cuSparse`

- `SUNMatDestroy_cuSparse`

- `SUNMatZero_cuSparse`

- `SUNMatCopy_cuSparse`

- `SUNMatScaleAdd_cuSparse` – performs $A = cA + B$, where A and B must have the same sparsity pattern

- `SUNMatScaleAddI_cuSparse` – performs $A = cA + I$, where the diagonal of A must be present

- `SUNMatMatvec_cuSparse`

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

SUNMatrix **SUNMatrix_cuSparse_NewCSR**(int M, int N, int NNZ, cusparseHandle_t cusp, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SUNMATRIX_CUSPARSE `SUNMatrix` that uses the CSR storage format. Its arguments are the number of rows and columns of the matrix, `M` and `N`, the number of nonzeros to be stored in the matrix, `NNZ`, and a valid `cusparseHandle_t`.

SUNMatrix **SUNMatrix_cuSparse_NewBlockCSR**(int nblocks, int blockrows, int blockcols, int blocknnz, cusparseHandle_t cusp, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SUNMATRIX_CUSPARSE `SUNMatrix` object that leverages the `SUNMAT_CUSPARSE_BCSR` storage format to store a block diagonal matrix where each block shares the same sparsity pattern. The blocks must be square. The function arguments are the number of blocks, `nblocks`, the number of rows, `blockrows`, the number of columns, `blockcols`, the number of nonzeros in each each block, `blocknnz`, and a valid `cusparseHandle_t`.

> **Warning:** The `SUNMAT_CUSPARSE_BCSR` format currently only supports square matrices, i.e., `blockrows == blockcols`.

SUNMatrix **SUNMatrix_cuSparse_MakeCSR**(cusparseMatDescr_t mat_descr, int M, int N, int NNZ, int *rowptrs, int *colind, *realtype* *data, cusparseHandle_t cusp, *SUNContext* sunctx)

This constructor function creates a SUNMATRIX_CUSPARSE `SUNMatrix` object from user provided pointers. Its arguments are a `cusparseMatDescr_t` that must have index base `CUSPARSE_INDEX_BASE_ZERO`, the number of rows and columns of the matrix, `M` and `N`, the number of nonzeros to be stored in the matrix, `NNZ`, and a valid `cusparseHandle_t`.

int **SUNMatrix_cuSparse_Rows**(*SUNMatrix* A)

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

int **SUNMatrix_cuSparse_Columns**(*SUNMatrix* A)

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

int **SUNMatrix_cuSparse_NNZ**(*SUNMatrix* A)

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

int **SUNMatrix_cuSparse_SparseType**(*SUNMatrix* A)

> This function returns the storage type (SUNMAT_CUSPARSE_CSR or SUNMAT_CUSPARSE_BCSR) for the sparse SUNMatrix.

realtype ***SUNMatrix_cuSparse_Data**(*SUNMatrix* A)

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

int ***SUNMatrix_cuSparse_IndexValues**(*SUNMatrix* A)

> This function returns a pointer to the index value array for the sparse SUNMatrix – for the CSR format this is an array of column indices for each nonzero entry. For the BCSR format this is an array of the column indices for each nonzero entry in the first block only.

int ***SUNMatrix_cuSparse_IndexPointers**(*SUNMatrix* A)

> This function returns a pointer to the index pointer array for the sparse SUNMatrix – for the CSR format this is an array of the locations of the first entry of each row in the data and indexvalues arrays, for the BCSR format this is an array of the locations of each row in the data and indexvalues arrays in the first block only.

int **SUNMatrix_cuSparse_NumBlocks**(*SUNMatrix* A)

> This function returns the number of matrix blocks.

int **SUNMatrix_cuSparse_BlockRows**(*SUNMatrix* A)

> This function returns the number of rows in a matrix block.

int **SUNMatrix_cuSparse_BlockColumns**(*SUNMatrix* A)

> This function returns the number of columns in a matrix block.

int **SUNMatrix_cuSparse_BlockNNZ**(*SUNMatrix* A)

> This function returns the number of nonzeros in each matrix block.

realtype ***SUNMatrix_cuSparse_BlockData**(*SUNMatrix* A, int blockidx)

> This function returns a pointer to the location in the data array where the data for the block, blockidx, begins. Thus, blockidx must be less than SUNMatrix_cuSparse_NumBlocks(A). The first block in the SUNMatrix is index 0, the second block is index 1, and so on.

cusparseMatDescr_t **SUNMatrix_cuSparse_MatDescr**(*SUNMatrix* A)

> This function returns the cusparseMatDescr_t object associated with the matrix.

int **SUNMatrix_cuSparse_CopyToDevice**(*SUNMatrix* A, *realtype* *h_data, int *h_idxptrs, int *h_idxvals)

> This functions copies the matrix information to the GPU device from the provided host arrays. A user may provide NULL for any of h_data, h_idxptrs, or h_idxvals to avoid copying that information.
>
> The function returns SUNMAT_SUCCESS if the copy operation(s) were successful, or a nonzero error code otherwise.

int **SUNMatrix_cuSparse_CopyFromDevice**(*SUNMatrix* A, *realtype* *h_data, int *h_idxptrs, int *h_idxvals)

> This functions copies the matrix information from the GPU device to the provided host arrays. A user may provide NULL for any of h_data, h_idxptrs, or h_idxvals to avoid copying that information. Otherwise:
>
> - The h_data array must be at least SUNMatrix_cuSparse_NNZ(A)*sizeof(realtype) bytes.
> - The h_idxptrs array must be at least (SUNMatrix_cuSparse_BlockDim(A)+1)*sizeof(int) bytes.
> - The h_idxvals array must be at least (SUNMatrix_cuSparse_BlockNNZ(A))*sizeof(int) bytes.
>
> The function returns SUNMAT_SUCCESS if the copy operation(s) were successful, or a nonzero error code otherwise.

int **SUNMatrix_cuSparse_SetFixedPattern**(*SUNMatrix* A, *booleantype* yesno)

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

int **SUNMatrix_cuSparse_SetKernelExecPolicy**(*SUNMatrix* A, SUNCudaExecPolicy *exec_policy)

> This function sets the execution policies which control the kernel parameters utilized when launching the CUDA kernels. By default the matrix is setup to use a policy which tries to leverage the structure of the matrix. See §6.10.2 for more information about the *SUNCudaExecPolicy* class.

7.7.3 SUNMATRIX_CUSPARSE Usage Notes

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

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

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

7.8 The SUNMATRIX_SPARSE Module

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

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

A diagram of the underlying data representation in a sparse matrix is shown in Fig. 7.2. A more complete description of the parts of this *content* field is given below:

- `M` - number of rows

- `N` - number of columns

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

- `NP` - number of index pointers (e.g. number of column pointers for CSC matrix). For CSC matrices `NP=N`, and for CSR matrices `NP=M`. This value is set automatically at construction based the input choice 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 SUNMATRIX_SPARSE content structure for user convenience, to provide a more intuitive interface to the CSC and CSR sparse matrix data structures. They are set automatically when creating a sparse `SUNMatrix`, based on the sparse matrix storage type.

- `rowvals` - pointer to `indexvals` when `sparsetype` is `CSC_MAT`, otherwise set to NULL.

- `colptrs` - pointer to `indexptrs` when `sparsetype` is `CSC_MAT`, otherwise set to NULL.

- `colvals` - pointer to `indexvals` when `sparsetype` is `CSR_MAT`, otherwise set to NULL.

- `rowptrs` - pointer to `indexptrs` when `sparsetype` is `CSR_MAT`, otherwise set to NULL.

For example, the 5×4 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 as a CSC matrix in this structure as either

```
M = 5;
N = 4;
NNZ = 8;
NP = N;
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4};
indexptrs = {0, 2, 4, 5, 8};
```

or

```
M = 5;
N = 4;
NNZ = 10;
NP = N;
```

```
data = {3.0, 1.0, 3.0, 7.0, 1.0, 2.0, 9.0, 5.0, *, *};
sparsetype = CSC_MAT;
indexvals = {1, 3, 0, 2, 0, 1, 3, 4, *, *};
indexptrs = {0, 2, 4, 5, 8};
```

where the first has no unused space, and the second has additional storage (the entries marked with * may contain any values). Note in both cases that the final value in `indexptrs` is 8, indicating the total number of nonzero entries in the matrix.

Similarly, in CSR format, the same matrix could be stored as

```
M = 5;
N = 4;
NNZ = 8;
NP = M;
data = {3.0, 1.0, 3.0, 2.0, 7.0, 1.0, 9.0, 5.0};
sparsetype = CSR_MAT;
indexvals = {1, 2, 0, 3, 1, 0, 3, 3};
indexptrs = {0, 2, 4, 5, 7, 8};
```

The header file to be included when using this module is `sunmatrix/sunmatrix_sparse.h`.

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

SM_CONTENT_S(A)

> This macro gives access to the contents of the sparse `SUNMatrix` A.
>
> The assignment `A_cont = SM_CONTENT_S(A)` sets `A_cont` to be a pointer to the sparse `SUNMatrix` content structure.
>
> Implementation:
>
> ```
> #define SM_CONTENT_S(A)   ( (SUNMatrixContent_Sparse)(A->content) )
> ```

SM_ROWS_S(A)

> Access the number of rows in the sparse `SUNMatrix` A.
>
> This may be used either to retrieve or to set the value. For example, the assignment `A_rows = SM_ROWS_S(A)` sets `A_rows` to be the number of rows in the matrix A. Similarly, the assignment `SM_ROWS_S(A) = A_rows` sets the number of columns in A to equal `A_rows`.
>
> Implementation:
>
> ```
> #define SM_ROWS_S(A)   ( SM_CONTENT_S(A)->M )
> ```

SM_COLUMNS_S(A)

> Access the number of columns in the sparse `SUNMatrix` A. As with `SM_ROWS_S`, this may be used either to retrieve or to set the value.
>
> Implementation:
>
> ```
> #define SM_COLUMNS_S(A)   ( SM_CONTENT_S(A)->N )
> ```
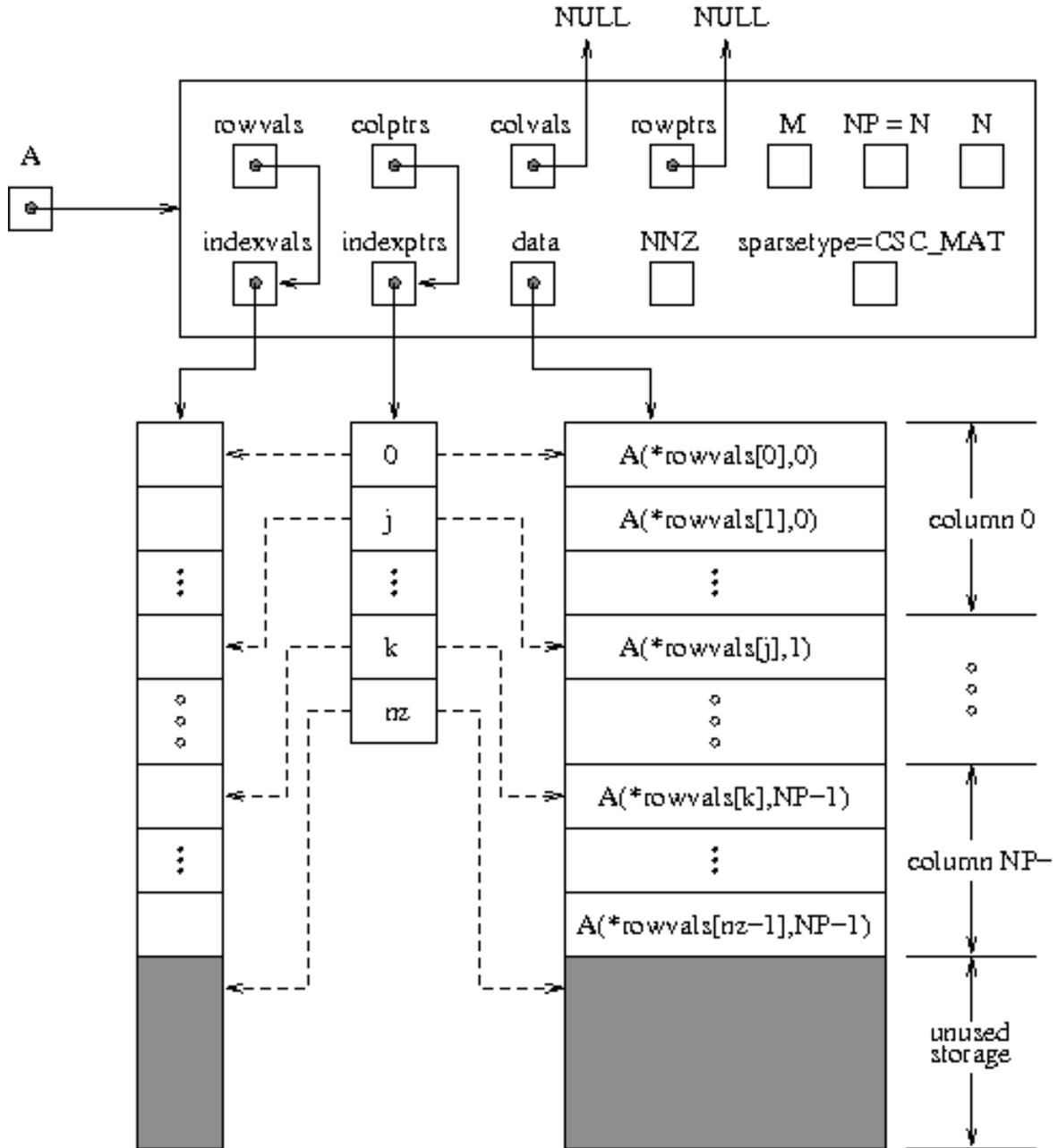
Fig. 7.2: Diagram of the storage for a compressed-sparse-column matrix of type SUNMATRIX_SPARSE: Here `A` is an $M \times N$ sparse CSC matrix with storage for up to `NNZ` nonzero entries (the allocated length of both `data` and `indexvals`). The entries in `indexvals` may assume values from `0` to `M-1`, corresponding to the row index (zero-based) of each nonzero value. The entries in `data` contain the values of the nonzero entries, with the row `i`, column `j` entry of `A` (again, zero-based) denoted as `A(i,j)`. The `indexptrs` array contains `N+1` entries; the first `N` denote the starting index of each column within the `indexvals` and `data` arrays, while the final entry points one past the final nonzero entry. Here, although `NNZ` values are allocated, only `nz` are actually filled in; the greyed-out portions of `data` and `indexvals` indicate extra allocated space.

SM_NNZ_S(A)

> Access the allocated number of nonzeros in the sparse SUNMatrix *A*. As with SM_ROWS_S, this may be used either to retrieve or to set the value.
>
> Implementation:
>
> ```
> #define SM_NNZ_S(A)    ( SM_CONTENT_S(A)->NNZ )
> ```

SM_NP_S(A)

> Access the number of index pointers NP in the sparse SUNMatrix *A*. As with SM_ROWS_S, this may be used either to retrieve or to set the value.
>
> Implementation:
>
> ```
> #define SM_NP_S(A)    ( SM_CONTENT_S(A)->NP )
> ```

SM_SPARSETYPE_S(A)

> Access the sparsity type parameter in the sparse SUNMatrix *A*. As with SM_ROWS_S, this may be used either to retrieve or to set the value.
>
> Implementation:
>
> ```
> #define SM_SPARSETYPE_S(A)    ( SM_CONTENT_S(A)->sparsetype )
> ```

SM_DATA_S(A)

> This macro gives access to the `data` pointer for the matrix entries.
>
> The assignment `A_data = SM_DATA_S(A)` sets `A_data` to be a pointer to the first component of the data array for the sparse SUNMatrix A. The assignment `SM_DATA_S(A) = A_data` sets the data array of *A* to be `A_data` by storing the pointer `A_data`.
>
> Implementation:
>
> ```
> #define SM_DATA_S(A)    ( SM_CONTENT_S(A)->data )
> ```

SM_INDEXVALS_S(A)

> This macro gives access to the `indexvals` pointer for the matrix entries.
>
> The assignment `A_indexvals = SM_INDEXVALS_S(A)` sets `A_indexvals` to be a pointer to the array of index values (i.e. row indices for a CSC matrix, or column indices for a CSR matrix) for the sparse SUNMatrix *A*.
>
> Implementation:
>
> ```
> #define SM_INDEXVALS_S(A)    ( SM_CONTENT_S(A)->indexvals )
> ```

SM_INDEXPTRS_S(A)

> This macro gives access to the `indexptrs` pointer for the matrix entries.
>
> The assignment `A_indexptrs = SM_INDEXPTRS_S(A)` sets `A_indexptrs` to be a pointer to the array of index pointers (i.e. the starting indices in the data/indexvals arrays for each row or column in CSR or CSC formats, respectively).
>
> Implementation:
>
> ```
> #define SM_INDEXPTRS_S(A)    ( SM_CONTENT_S(A)->indexptrs )
> ```

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

SUNMatrix **SUNSparseMatrix**(*sunindextype* M, *sunindextype* N, *sunindextype* NNZ, int sparsetype, *SUNContext* sunctx)

> This constructor function creates and allocates memory for a sparse SUNMatrix. Its arguments are the number of rows and columns of the matrix, *M* and *N*, the maximum number of nonzeros to be stored in the matrix, *NNZ*, and a flag *sparsetype* indicating whether to use CSR or CSC format (valid choices are CSR_MAT or CSC_MAT).

SUNMatrix **SUNSparseFromDenseMatrix**(*SUNMatrix* A, *realtype* droptol, int sparsetype)

> This constructor function creates a new sparse matrix from an existing SUNMATRIX_DENSE object by copying all values with magnitude larger than *droptol* into the sparse matrix structure.
>
> Requirements:
>
> - *A* must have type SUNMATRIX_DENSE
>
> - *droptol* must be non-negative
>
> - *sparsetype* must be either CSC_MAT or CSR_MAT
>
> The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

SUNMatrix **SUNSparseFromBandMatrix**(*SUNMatrix* A, *realtype* droptol, int sparsetype)

> This constructor function creates a new sparse matrix from an existing SUNMATRIX_BAND object by copying all values with magnitude larger than *droptol* into the sparse matrix structure.
>
> Requirements:
>
> - *A* must have type SUNMATRIX_BAND
>
> - *droptol* must be non-negative
>
> - *sparsetype* must be either CSC_MAT or CSR_MAT.
>
> The function returns NULL if any requirements are violated, or if the matrix storage request cannot be satisfied.

int **SUNSparseMatrix_Realloc**(*SUNMatrix* A)

> This function reallocates internal storage arrays in a sparse matrix so that the resulting sparse matrix has no wasted space (i.e. the space allocated for nonzero entries equals the actual number of nonzeros, indexptrs[NP]). Returns 0 on success and 1 on failure (e.g. if the input matrix is not sparse).

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

> This function prints the content of a sparse SUNMatrix to the output stream specified by outfile. Note: stdout or stderr may be used as arguments for outfile to print directly to standard output or standard error, respectively.

sunindextype **SUNSparseMatrix_Rows**(*SUNMatrix* A)

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

sunindextype **SUNSparseMatrix_Columns**(*SUNMatrix* A)

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

sunindextype **SUNSparseMatrix_NNZ**(*SUNMatrix* A)

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

sunindextype **SUNSparseMatrix_NP**(*SUNMatrix* A)

> This function returns the number of index pointers for the sparse SUNMatrix (the indexptrs array has NP+1 entries).

int **SUNSparseMatrix_SparseType**(*SUNMatrix* A)

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

---

realtype ***SUNSparseMatrix_Data**(*SUNMatrix* A)

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

sunindextype ***SUNSparseMatrix_IndexValues**(*SUNMatrix* A)

    This function returns a pointer to index value array for the sparse SUNMatrix – for CSR format this is the column index for each nonzero entry, for CSC format this is the row index for each nonzero entry.

sunindextype ***SUNSparseMatrix_IndexPointers**(*SUNMatrix* A)

    This function returns a pointer to the index pointer array for the sparse SUNMatrix – for CSR format this is the location of the first entry of each row in the `data` and `indexvalues` arrays, for CSC format this is the location of the first entry of each column.

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

7.9 The SUNMATRIX_SLUNRLOC Module

The SUNMATRIX_SLUNRLOC module is an interface to the `SuperMatrix` structure provided by the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li and collaborators [7, 32, 45, 46]. It is designed to be used with the SuperLU_DIST SUNLinearSolver module discussed in §8.15. To this end, it defines the `content` field of SUNMatrix to be the following structure:

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

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

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

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

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

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

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

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

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

7.9.1 SUNMATRIX_SLUNRLOC Functions

The SUNMATRIX_SLUNRLOC module provides the following user-callable routines:

SUNMatrix **SUNMatrix_SLUNRloc**(SuperMatrix *Asuper, gridinfo_t *grid, *SUNContext* sunctx)

> This constructor function creates and allocates memory for a SUNMATRIX_SLUNRLOC object. Its arguments are a fully-allocated SuperLU_DIST SuperMatrix with `Stype = SLU_NR_loc`, `Dtype = SLU_D`, `Mtype = SLU_GE` and an initialized SuperLU_DIST 2D process grid structure. It returns a `SUNMatrix` object if `Asuper` is compatible else it returns `NULL`.

void **SUNMatrix_SLUNRloc_Print**(*SUNMatrix* A, FILE *fp)

> This function prints the underlying `SuperMatrix` content. It is useful for debugging. Its arguments are the `SUNMatrix` object and a `FILE` pointer to print to. It returns void.

SuperMatrix ***SUNMatrix_SLUNRloc_SuperMatrix**(*SUNMatrix* A)

> This function returns the underlying `SuperMatrix` of `A`. Its only argument is the `SUNMatrix` object to access.

gridinfo_t ***SUNMatrix_SLUNRloc_ProcessGrid**(*SUNMatrix* A)

> This function returns the SuperLU_DIST 2D process grid associated with `A`. Its only argument is the `SUNMatrix` object to access.

booleantype **SUNMatrix_SLUNRloc_OwnData**(*SUNMatrix* A)

> This function returns true if the `SUNMatrix` object is responsible for freeing the underlying `SuperMatrix`, otherwise it returns false. Its only argument is the `SUNMatrix` object to access.

The SUNMATRIX_SLUNRLOC module also defines implementations of all generic `SUNMatrix` operations listed in §7.2:

- `SUNMatGetID_SLUNRloc` – returns SUNMATRIX_SLUNRLOC

- `SUNMatClone_SLUNRloc`

- `SUNMatDestroy_SLUNRloc`

- `SUNMatSpace_SLUNRloc` – this only returns information for the storage within the matrix interface, i.e. storage for `row_to_proc`

- `SUNMatZero_SLUNRloc`

- `SUNMatCopy_SLUNRloc`

- `SUNMatScaleAdd_SLUNRloc` – performs $A = cA + B$, where A and B must have the same sparsity pattern

- `SUNMatScaleAddI_SLUNRloc` – performs $A = cA + I$, where the diagonal of A must be present

- `SUNMatMatvecSetup_SLUNRloc` – initializes the SuperLU_DIST parallel communication structures needed to perform a matrix-vector product; only needs to be called before the first call to *SUNMatMatvec()* or if the matrix changed since the last setup

- `SUNMatMatvec_SLUNRloc`

7.10 The SUNMATRIX_GINKGO Module

New in version 6.4.0.

The SUNMATRIX_GINKGO implementation of the `SUNMatrix` API provides an interface to the matrix data structure for the Ginkgo linear algebra library [10]. Ginkgo provides several different matrix formats and linear solvers which can run on a variety of hardware, such as NVIDIA, AMD, and Intel GPUs as well as multicore CPUs. Since Ginkgo is a modern C++ library, SUNMATRIX_GINKGO is also written in modern C++ (it requires C++14). Unlike most other SUNDIALS modules, it is a header only library. To use the SUNMATRIX_GINKGO `SUNMatrix`, users will need to include `sunmatrix/sunmatrix_ginkgo.hpp`. More instructions on building SUNDIALS with Ginkgo enabled are given in §11.1.4. For instructions on building and using Ginkgo itself, refer to the Ginkgo website and documentation.

Note: It is assumed that users of this module are aware of how to use Ginkgo. This module does not try to encapsulate Ginkgo matrices, rather it provides a lightweight iteroperability layer between Ginkgo and SUNDIALS.

The SUNMATRIX_GINKGO module is defined by the `sundials::ginkgo::Matrix` templated class:

```
template<typename GkoMatType>
class Matrix : public sundials::impl::BaseMatrix, public sundials::ConvertibleTo<SUNMatrix>;
```

7.10.1 Compatible `N_Vectors`

The `N_Vector` to use with the SUNLINEARSOLVER_GINKGO module depends on the `gko::Executor` utilized. That is, when using the `gko::CudaExecutor` you should use a CUDA capable `N_Vector` (e.g., §6.10), `gko::HipExecutor` goes with a HIP capable `N_Vector` (e.g., §6.11), `gko::DpcppExecutor` goes with a DPC++/SYCL capable `N_Vector` (e.g., §6.12), and `gko::OmpExecutor` goes with a CPU based N_Vector (e.g., §6.6). Specifically, what makes a `N_Vector` compatible with different Ginkgo executors is where they store the data. The GPU enabled Ginkgo executors need the data to reside on the GPU, so the `N_Vector` must implement *N_VGetDeviceArray-Pointer()* and keep the data in GPU memory. The CPU-only enabled Ginkgo executors (e.g, `gko::OmpExecutor` and `gko::ReferenceExecutor`) need data to reside on the CPU and will use `N_VGetArraryPointer()` to access the `N_Vector` data.

7.10.2 Using SUNMATRIX_GINKGO

To use the SUNMATRIX_GINKGO module, we begin by creating an instance of a Ginkgo matrix using Ginkgo's API. For example, below we create a Ginkgo sparse matrix that uses the CSR storage format and then fill the diagonal of the matrix with ones to make an identity matrix:

```
auto gko_matrix{gko::matrix::Csr<sunrealtype, sunindextype>::create(gko_exec, matrix_dim)};
gko_matrix->read(gko::matrix_data<sunrealtype, sunindextype>::diag(matrix_dim, 1.0));
```

After we have a Ginkgo matrix object, we wrap it in an instance of the `sundials::ginkgo::Matrix` class. This object can be provided to other SUNDIALS functions that expect a `SUNMatrix` object via implicit conversion, or the `Convert()` method:

```
sundials::ginkgo::Matrix<gko::matrix::Csr> matrix{gko_matrix, sunctx};
SUNMatrix I1 = matrix.Convert(); // explicit conversion to SUNMatrix
SUNMatrix I2 = matrix;  // implicit conversion to SUNMatrix
```

No further interaction with `matrix` is required from this point, and it is possible to to use the `SUNMatrix` API operating on `I1` or `I2` (or if needed, via Ginkgo operations on `gko_matrix`).

> **Warning:** *SUNMatDestroy()* should never be called on a `SUNMatrix` that was created via conversion from a `sundials::ginkgo::Matrix`. Doing so may result in a double free.

7.10.3 SUNMATRIX_GINKGO API

In this section we list the public API of the `sundials::ginkgo::Matrix` class.

template<typename **GkoMatType**>
class **Matrix** : public sundials::impl::BaseMatrix, public sundials::ConvertibleTo<SUNMatrix>

> **Matrix**() = default
>
>> Default constructor - means the matrix must be copied or moved to.
>
> **Matrix**(std::shared_ptr<*GkoMatType*> gko_mat, SUNContext sunctx)
>
>> Constructs a Matrix from an existing Ginkgo matrix object.
>>
>>> **Parameters**
>>>
>>>> • **gko_mat** – A Ginkgo matrix object
>>>>
>>>> • **sunctx** – The SUNDIALS simulation context object (*SUNContext*)
>
> **Matrix**(*Matrix* &&that_matrix) noexcept
>
>> Move constructor.
>
> **Matrix**(const *Matrix* &that_matrix)
>
>> Copy constructor (performs a deep copy).
>
> *Matrix* &**operator=**(*Matrix* &&rhs) noexcept
>
>> Move assignment.
>
> *Matrix* &**operator=**(const *Matrix* &rhs)
>
>> Copy assignment clones the `gko::matrix` and *SUNMatrix*. This is a deep copy (i.e. a new data array is created).
>
> virtual **~Matrix**() = default;
>
>> Default destructor.
>
> std::shared_ptr<*GkoMatType*> **GkoMtx**() const
>
>> Get the underlying Ginkgo matrix object.
>
> std::shared_ptr<const gko::Executor> **GkoExec**() const
>
>> Get the `gko::Executor` associated with the Ginkgo matrix.
>
> const gko::dim<2> &**GkoSize**() const
>
>> Get the size, i.e. `gko::dim`, for the Ginkgo matrix.
>
> operator **SUNMatrix**() override
>
>> Implicit conversion to a *SUNMatrix*.
>
> operator **SUNMatrix**() const override
>
>> Implicit conversion to a *SUNMatrix*.
>
> SUNMatrix **Convert**() override
>
>> Explicit conversion to a *SUNMatrix*.
>
> SUNMatrix **Convert**() const override
>
>> Explicit conversion to a *SUNMatrix*.

7.11 The SUNMATRIX_KOKKOSDENSE Module

New in version 6.4.0.

The SUNMATRIX_KOKKOSDENSE *SUNMatrix* implementation provides a data structure for dense and dense batched (block-diagonal) matrices using Kokkos [28, 55] and KokkosKernels [54] to support a variety of backends including serial, OpenMP, CUDA, HIP, and SYCL. Since Kokkos is a modern C++ library, the module is also written in modern C++ (it requires C++14) as a header only library. To utilize this `SUNMatrix` users will need to include `sunmatrix/sunmatrix_kokkosdense.hpp`. More instructions on building SUNDIALS with Kokkos and KokkosKernels enabled are given in §11.1.4. For instructions on building and using Kokkos and KokkosKernels, refer to the Kokkos and KokkosKernels. documentation.

7.11.1 Using SUNMATRIX_KOKKOSDENSE

The SUNMATRIX_KOKKOSDENSE module is defined by the `DenseMatrix` templated class in the `sundials::kokkos` namespace:

```
template<class ExecutionSpace = Kokkos::DefaultExecutionSpace,
         class MemorySpace = typename ExecSpace::memory_space>
class DenseMatrix : public sundials::impl::BaseMatrix,
                    public sundials::ConvertibleTo<SUNMatrix>
```

To use the SUNMATRIX_KOKKOSDENSE module, we begin by constructing an instance of the Kokkos dense matrix e.g.,

```
// Single matrix using the default execution space
sundials::kokkos::DenseMatrix<> A{rows, cols, sunctx};

// Batched (block-diagonal) matrix using the default execution space
sundials::kokkos::DenseMatrix<> Abatch{blocks, rows, cols, sunctx};

// Batched (block-diagonal) matrix using the Cuda execution space
sundials::kokkos::DenseMatrix<Kokkos::Cuda> Abatch{blocks, rows, cols, sunctx};

// Batched (block-diagonal) matrix using the Cuda execution space and
// a non-default execution space instance
sundials::kokkos::DenseMatrix<Kokkos::Cuda> Abatch{blocks, rows, cols,
                                                   exec_space_instance,
                                                   sunctx};
```

Instances of the `DenseMatrix` class are implicitly or explicitly (using the *Convert()* method) convertible to a *SUNMatrix* e.g.,

```
sundials::kokkos::DenseMatrix<> A{rows, cols, sunctx};
SUNMatrix B = A;            // implicit conversion to SUNMatrix
SUNMatrix C = A.Convert(); // explicit conversion to SUNMatrix
```

No further interaction with a `DenseMatrix` is required from this point, and it is possible to use the *SUNMatrix* API to operate on B or C.

Warning: *SUNMatDestroy()* should never be called on a SUNMatrix that was created via conversion from a `sundials::kokkos::DenseMatrix`. Doing so may result in a double free.

The underlying `DenseMatrix` can be extracted from a `SUNMatrix` using *GetDenseMat()* e.g.,

```
auto A_dense_mat = GetDenseMat<>(A_sunmat);
```

The SUNMATRIX_KOKKOSDENSE module is compatible with the NVECTOR_KOKKOS vector module (see §6.14) and SUNLINEARSOLVER_KOKKOSDENSE linear solver module (see §8.19).

7.11.2 SUNMATRIX_KOKKOSDENSE API

In this section we list the public API of the `sundials::kokkos::DenseMatrix` class.

template<class **ExeccutionSpace** = Kokkos::DefaultExecutionSpace, class **MemorySpace** = typename *ExecSpace*::memory_space>
class **DenseMatrix** : public sundials::impl::BaseMatrix, public sundials::ConvertibleTo<SUNMatrix>

> **DenseMatrix**() = default
>
> > Default constructor – the matrix must be copied or moved to.
>
> **DenseMatrix**(size_type rows, size_type cols, SUNContext sunctx)
>
> > Constructs a single DenseMatrix using the default execution space instance.
> >
> > > **Parameters**
> > >
> > > - **rows** – number of matrix rows
> > >
> > > - **cols** – number of matrix columns
> > >
> > > - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **DenseMatrix**(size_type rows, size_type cols, exec_space ex, SUNContext sunctx)
>
> > Constructs a single DenseMatrix using the provided execution space instance.
> >
> > > **Parameters**
> > >
> > > - **rows** – number of matrix rows
> > >
> > > - **cols** – number of matrix columns
> > >
> > > - **exec_space** – a *ExecSpace* instance
> > >
> > > - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **DenseMatrix**(size_type blocks, size_type block_rows, size_type block_cols, SUNContext sunctx)
>
> > Constructs a batched (block-diagonal) DenseMatrix using the default execution space instance.
> >
> > > **Parameters**
> > >
> > > - **blocks** – number of matrix blocks
> > >
> > > - **block_rows** – number of rows in a block
> > >
> > > - **block_cols** – number of columns in a block
> > >
> > > - **sunctx** – the SUNDIALS simulation context object (*SUNContext*)
>
> **DenseMatrix**(size_type blocks, size_type block_rows, size_type block_cols, exec_space ex, SUNContext sunctx)
>
> > Constructs a batched (block-diagonal) DenseMatrix using the provided execution space instance.
> >
> > > **Parameters**
> > >
> > > - **blocks** – number of matrix blocks

- **block_rows** – number of rows in a block
- **block_cols** – number of columns in a block
- **exec_space** – a *ExecSpace* instance
- **sunctx** – the SUNDIALS simulation context object (*SUNContext*)

DenseMatrix(*DenseMatrix* &&that_matrix) noexcept

Move constructor.

DenseMatrix(const *DenseMatrix* &that_matrix)

Copy constructor. This creates a shallow clone of the Matrix, i.e., it creates a new Matrix with the same properties, such as size, but it does not copy the data.

DenseMatrix &**operator=**(*DenseMatrix* &&rhs) noexcept

Move assignment.

DenseMatrix &**operator=**(const *DenseMatrix* &rhs)

Copy assignment. This creates a shallow clone of the Matrix, i.e., it creates a new Matrix with the same properties, such as size, but it does not copy the data.

virtual **~DenseMatrix**() = default;

Default destructor.

exec_space **ExecSpace**()

Get the execution space instance used by the matrix.

view_type **View**()

Get the underlying Kokkos view with extents {blocks, block_rows, block_cols}.

size_type **Blocks**()

Get the number of blocks i.e., extent(0).

size_type **BlockRows**()

Get the number of rows in a block i.e., extent(1).

size_type **BlockCols**()

Get the number of columns in a block i.e., extent(2).

size_type **Rows**()

Get the number of rows in the block-diagonal matrix i.e., extent(0) * extent(1).

size_type **Cols**()

Get the number of columns in the block-diagonal matrix i.e., extent(0) * extent(2).

operator SUNMatrix() override

Implicit conversion to a *SUNMatrix*.

operator SUNMatrix() const override

Implicit conversion to a *SUNMatrix*.

SUNMatrix **Convert**() override

Explicit conversion to a *SUNMatrix*.

SUNMatrix **Convert**() const override

Explicit conversion to a *SUNMatrix*.

template<class **ExecutionSpace** = Kokkos::DefaultExecutionSpace, class **MemorySpace** = typename ExecSpace::memory_space>

inline *DenseMatrix*<MatrixType> ***GetDenseMat**(SUNMatrix A)

> Get the dense matrix wrapped by a SUNMatrix

7.12 SUNMATRIX Examples

There are `SUNMatrix` examples that may be installed for each implementation, that make use of the functions in `test_-sunmatrix.c`. These example functions show simple usage of the `SUNMatrix` family of functions. The inputs to the examples depend on the matrix type, and are output to `stdout` if the example is run without the appropriate number of command-line arguments.

The following is a list of the example functions in `test_sunmatrix.c`:

- `Test_SUNMatGetID`: Verifies the returned matrix ID against the value that should be returned.

- `Test_SUNMatClone`: Creates clone of an existing matrix, copies the data, and checks that their values match.

- `Test_SUNMatZero`: Zeros out an existing matrix and checks that each entry equals 0.0.

- `Test_SUNMatCopy`: Clones an input matrix, copies its data to a clone, and verifies that all values match.

- `Test_SUNMatScaleAdd`: Given an input matrix A and an input identity matrix I, this test clones and copies A to a new matrix B, computes $B = -B + B$, and verifies that the resulting matrix entries equal 0. Additionally, if the matrix is square, this test clones and copies A to a new matrix D, clones and copies I to a new matrix C, computes $D = D + I$ and $C = C + A$ using *SUNMatScaleAdd()*, and then verifies that $C = D$.

- `Test_SUNMatScaleAddI`: Given an input matrix A and an input identity matrix I, this clones and copies I to a new matrix B, computes $B = -B + I$ using *SUNMatScaleAddI()*, and verifies that the resulting matrix entries equal 0.

- `Test_SUNMatMatvecSetup`: verifies that *SUNMatMatvecSetup()* can be called.

- `Test_SUNMatMatvec` Given an input matrix A and input vectors x and y such that $y = Ax$, this test has different behavior depending on whether A is square. If it is square, it clones and copies A to a new matrix B, computes $B = 3B + I$ using *SUNMatScaleAddI()*, clones y to new vectors w and z, computes $z = Bx$ using *SUNMatMatvec()*, computes $w = 3y + x$ using `N_VLinearSum`, and verifies that $w == z$. If A is not square, it just clones y to a new vector z, *computes :math:`z=Ax`* using *SUNMatMatvec()*, and verifies that $y = z$.

- `Test_SUNMatSpace`: verifies that *SUNMatSpace()* can be called, and outputs the results to `stdout`.

7.13 SUNMatrix functions used by CVODE

In Table 7.2, we list the matrix functions in the `SUNMatrix` module used within the CVODE package. The table also shows, for each function, which of the code modules uses the function. The main CVODE integrator does not call any `SUNMatrix` functions directly, so the table columns are specific to the CVLS interface and the CVBANDPRE and CVBBDPRE preconditioner modules. We further note that the CVLS interface only utilizes these routines when supplied with a *matrix-based* linear solver, i.e., the `SUNMatrix` object passed to *CVodeSetLinearSolver()* was not `NULL`.

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

Table 7.2: List of matrix functions usage by CVODE code modules

	CVLS	CVBANDPRE	CVBBDPRE
SUNMatClone()	x		
SUNMatDestroy()	x	x	x
SUNMatZero()	x	x	x
SUNMatGetID()	x		
SUNMatCopy()	x	x	x
SUNMatScaleAddI()	x	x	x
SUNMatSpace()	†	†	†

The matrix functions listed with a † symbol are optionally used, in that these are only called if they are implemented in the SUNMatrix module that is being used (i.e. their function pointers are non-NULL). The matrix functions listed in §7.1 that are *not* used by CVODE are: *SUNMatScaleAdd()* and *SUNMatMatvec()*. Therefore a user-supplied SUNMatrix module for CVODE could omit these functions.

We note that the CVBANDPRE and CVBBDPRE preconditioner modules are hard-coded to use the SUNDIALS-supplied band SUNMatrix type, so the most useful information above for user-supplied SUNMatrix implementations is the column relating the CVLS requirements.

Chapter 8

Linear Algebraic Solvers

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

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

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

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

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

where

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

and where

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

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

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

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

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

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

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

For users interested in providing their own SUNLinSol module, the following section presents the SUNLinSol API and its implementation beginning with the definition of SUNLinSol functions in §8.1.1 – §8.1.3. This is followed by the definition of functions supplied to a linear solver implementation in §8.1.4. The linear solver return codes are described in Table 8.1. The `SUNLinearSolver` type and the generic SUNLinSol module are defined in §8.1.6. §8.1.8 lists the requirements for supplying a custom SUNLinSol module and discusses some intended use cases. Users wishing to supply their own SUNLinSol module are encouraged to use the SUNLinSol implementations provided with SUNDIALS as a template for supplying custom linear solver modules. The section that then follows describes the SUNLinSol functions required by this SUNDIALS package, and provides additional package specific details. Then the remaining sections of this chapter present the SUNLinSol modules provided with SUNDIALS.

8.1 The SUNLinearSolver API

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

8.1.1 SUNLinearSolver core functions

The core linear solver functions consist of two **required** functions: *SUNLinSolGetType()* returns the linear solver type, and *SUNLinSolSolve()* solves the linear system $Ax = b$.

The remaining **optional** functions return the solver ID (*SUNLinSolGetID()*), initialize the linear solver object once all solver-specific options have been set (*SUNLinSolInitialize()*), set up the linear solver object to utilize an updated matrix A (*SUNLinSolSetup()*), and destroy a linear solver object (*SUNLinSolFree()*).

SUNLinearSolver_Type **SUNLinSolGetType**(*SUNLinearSolver* LS)

>   Returns the type identifier for the linear solver *LS*.

>   **Return value:**

>>   • `SUNLINEARSOLVER_DIRECT (0)` – the SUNLinSol module requires a matrix, and computes an "exact" solution to the linear system defined by that matrix.

- SUNLINEARSOLVER_ITERATIVE (1) – the SUNLinSol module does not require a matrix (though one may be provided), and computes an inexact solution to the linear system using a matrix-free iterative algorithm. That is it solves the linear system defined by the package-supplied `ATimes` routine (see *SUNLinSolSetATimes()* below), even if that linear system differs from the one encoded in the matrix object (if one is provided). As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.

- SUNLINEARSOLVER_MATRIX_ITERATIVE (2) – the SUNLinSol module requires a matrix, and computes an inexact solution to the linear system defined by that matrix using an iterative algorithm. That is it solves the linear system defined by the matrix object even if that linear system differs from that encoded by the package-supplied `ATimes` routine. As the solver computes the solution only inexactly (or may diverge), the linear solver should check for solution convergence/accuracy as appropriate.

- SUNLINEARSOLVER_MATRIX_EMBEDDED (3) – the SUNLinSol module sets up and solves the specified linear system at each linear solve call. Any matrix-related data structures are held internally to the linear solver itself, and are not provided by the SUNDIALS package.

Usage:

```
type = SUNLinSolGetType(LS);
```

Note: See §8.1.8.1 for more information on intended use cases corresponding to the linear solver type.

SUNLinearSolver_ID **SUNLinSolGetID**(*SUNLinearSolver* LS)

Returns a non-negative linear solver identifier (of type `int`) for the linear solver *LS*.

Return value:

Non-negative linear solver identifier (of type `int`), defined by the enumeration SUNLinearSolver_ID, with values shown in Table 8.2 and defined in the `sundials_linearsolver.h` header file.

Usage:

```
id = SUNLinSolGetID(LS);
```

Note: It is recommended that a user-supplied SUNLinearSolver return the SUNLINEARSOLVER_CUSTOM identifier.

---

int **SUNLinSolInitialize**(*SUNLinearSolver* LS)

Performs linear solver initialization (assuming that all solver-specific options have been set).

Return value:

Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

Usage:

```
retval = SUNLinSolInitialize(LS);
```

int **SUNLinSolSetup**(*SUNLinearSolver* LS, *SUNMatrix* A)

Performs any linear solver setup needed, based on an updated system SUNMatrix *A*. This may be called frequently (e.g., with a full Newton method) or infrequently (for a modified Newton method), based on the type of integrator and/or nonlinear solver requesting the solves.

Return value:

Zero for a successful call, a positive value for a recoverable failure, and a negative value for an unrecoverable failure. Ideally this should return one of the generic error codes listed in Table 8.1.

Usage:

```
retval = SUNLinSolSetup(LS, A);
```

int **SUNLinSolSolve**(*SUNLinearSolver* LS, *SUNMatrix* A, *N_Vector* x, *N_Vector* b, *realtype* tol)

This *required* function solves a linear system $Ax = b$.

Arguments:

- *LS* – a SUNLinSol object.

- *A* – a SUNMatrix object.

- *x* – an N_Vector object containing the initial guess for the solution of the linear system on input, and the solution to the linear system upon return.

- *b* – an N_Vector object containing the linear system right-hand side.

- *tol* – the desired linear solver tolerance.

Return value:

Zero for a successful call, a positive value for a recoverable failure, and a negative value for an unrecoverable failure. Ideally this should return one of the generic error codes listed in Table 8.1.

Notes:

Direct solvers: can ignore the *tol* argument.

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

Iterative solvers: (those that identify as SUNLINEARSOLVER_ITERATIVE or SUNLINEARSOLVER_-MATRIX_ITERATIVE) should attempt to solve to the specified tolerance *tol* in a weighted 2-norm. If the solver does not support scaling then it should just use a 2-norm.

Matrix-embedded solvers: should ignore the SUNMatrix input *A* as this will be NULL. It is assumed that within this function, the solver will call interface routines from the relevant SUNDIALS package to directly form the linear system matrix *A*, and then solve $Ax = b$ before returning with the solution x.

Usage:

```
retval = SUNLinSolSolve(LS, A, x, b, tol);
```

int **SUNLinSolFree**(*SUNLinearSolver* LS)

Frees memory allocated by the linear solver.

Return value:

Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

Usage:

```
retval = SUNLinSolFree(LS);
```

8.1.2 SUNLinearSolver "set" functions

The following functions supply linear solver modules with functions defined by the SUNDIALS packages and modify solver parameters. Only the routine for setting the matrix-vector product routine is required, and even then is only required for matrix-free linear solver modules. Otherwise, all other set functions are optional. SUNLinSol implementations that do not provide the functionality for any optional routine should leave the corresponding function pointer NULL instead of supplying a dummy routine.

int **SUNLinSolSetATimes**(*SUNLinearSolver* LS, void *A_data, *SUNATimesFn* ATimes)

> *Required for matrix-free linear solvers* (otherwise optional).

> Provides a *SUNATimesFn* function pointer, as well as a `void*` pointer to a data structure used by this routine, to the linear solver object *LS*. SUNDIALS packages call this function to set the matrix-vector product function to either a solver-provided difference-quotient via vector operations or a user-supplied solver-specific routine.

> **Return value:**

>> Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

> **Usage:**

>> ```
>> retval = SUNLinSolSetATimes(LS, A_data, ATimes);
>> ```

int **SUNLinSolSetPreconditioner**(*SUNLinearSolver* LS, void *P_data, *SUNPSetupFn* Pset, *SUNPSolveFn* Psol)

> This *optional* routine provides *SUNPSetupFn* and *SUNPSolveFn* function pointers that implement the preconditioner solves P_1^{-1} and P_2^{-1} from (8.2). This routine is called by a SUNDIALS package, which provides translation between the generic *Pset* and *Psol* calls and the package- or user-supplied routines.

> **Return value:**

>> Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

> **Usage:**

>> ```
>> retval = SUNLinSolSetPreconditioner(LS, Pdata, Pset, Psol);
>> ```

int **SUNLinSolSetScalingVectors**(*SUNLinearSolver* LS, *N_Vector* s1, *N_Vector* s2)

> This *optional* routine provides left/right scaling vectors for the linear system solve. Here, *s1* and *s2* are N_Vectors of positive scale factors containing the diagonal of the matrices S_1 and S_2 from (8.2), respectively. Neither vector needs to be tested for positivity, and a NULL argument for either indicates that the corresponding scaling matrix is the identity.

> **Return value:**

>> Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

> **Usage:**

>> ```
>> retval = SUNLinSolSetScalingVectors(LS, s1, s2);
>> ```

int **SUNLinSolSetZeroGuess**(*SUNLinearSolver* LS, *booleantype* onoff)

> This *optional* routine indicates if the upcoming `SUNlinSolSolve()` call will be made with a zero initial guess (SUNTRUE) or a non-zero initial guess (SUNFALSE).

> **Return value:**

Zero for a successful call, and a negative value for a failure. Ideally, this should return one of the generic error codes listed in Table 8.1.

Usage:

```
retval = SUNLinSolSetZeroGuess(LS, onoff);
```

Notes:

It is assumed that the initial guess status is not retained across calls to *SUNLinSolSolve()*. As such, the linear solver interfaces in each of the SUNDIALS packages call *SUNLinSolSetZeroGuess()* prior to each call to *SUNLinSolSolve()*.

8.1.3 SUNLinearSolver "get" functions

The following functions allow SUNDIALS packages to retrieve results from a linear solve. *All routines are optional.*

int **SUNLinSolNumIters**(*SUNLinearSolver* LS)

This *optional* routine should return the number of linear iterations performed in the most-recent "solve" call.

Usage:

```
its = SUNLinSolNumIters(LS);
```

realtype **SUNLinSolResNorm**(*SUNLinearSolver* LS)

This *optional* routine should return the final residual norm from the most-recent "solve" call.

Usage:

```
rnorm = SUNLinSolResNorm(LS);
```

N_Vector **SUNLinSolResid**(*SUNLinearSolver* LS)

If an iterative method computes the preconditioned initial residual and returns with a successful solve without performing any iterations (i.e., either the initial guess or the preconditioner is sufficiently accurate), then this *optional* routine may be called by the SUNDIALS package. This routine should return the N_Vector containing the preconditioned initial residual vector.

Usage:

```
rvec = SUNLinSolResid(LS);
```

Notes:

Since N_Vector is actually a pointer, and the results are not modified, this routine should *not* require additional memory allocation. If the SUNLinSol object does not retain a vector for this purpose, then this function pointer should be set to NULL in the implementation.

sunindextype **SUNLinSolLastFlag**(*SUNLinearSolver* LS)

This *optional* routine should return the last error flag encountered within the linear solver. Although not called by the SUNDIALS packages directly, this may be called by the user to investigate linear solver issues after a failed solve.

Usage:

```
lflag = SUNLinLastFlag(LS);
```

int **SUNLinSolSpace**(*SUNLinearSolver* LS, long int *lenrwLS, long int *leniwLS)

   This *optional* routine should return the storage requirements for the linear solver *LS*:

   - *lrw* is a `long int` containing the number of realtype words

   - *liw* is a `long int` containing the number of integer words.

   The return value is an integer flag denoting success/failure of the operation.

   This function is advisory only, for use by users to help determine their total space requirements.

   Usage:

   ```
   retval = SUNLinSolSpace(LS, &lrw, &liw);
   ```

8.1.4 Functions provided by SUNDIALS packages

To interface with SUNLinSol modules, the SUNDIALS packages supply a variety of routines for evaluating the matrix-vector product, and setting up and applying the preconditioner. These package-provided routines translate between the user-supplied ODE, DAE, or nonlinear systems and the generic linear solver API. The function types for these routines are defined in the header file `sundials/sundials_iterative.h`, and are described below.

typedef int (*__SUNATimesFn__)(void *A_data, *N_Vector* v, *N_Vector* z)

   Computes the action of a matrix on a vector, performing the operation $z \leftarrow Av$. Memory for z will already be allocated prior to calling this function. The parameter *A_data* is a pointer to any information about A which the function needs in order to do its job. The vector v should be left unchanged.

   Return value:

      Zero for a successful call, and non-zero upon failure.

typedef int (*__SUNPSetupFn__)(void *P_data)

   Sets up any requisite problem data in preparation for calls to the corresponding *SUNPSolveFn*.

   Return value:

      Zero for a successful call, and non-zero upon failure.

typedef int (*__SUNPSolveFn__)(void *P_data, *N_Vector* r, *N_Vector* z, *realtype* tol, int lr)

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

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

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

   Return value:

      Zero for a successful call, a negative value for an unrecoverable failure condition, or a positive value for a recoverable failure condition (thus the calling routine may reattempt the solution after updating preconditioner data).

8.1.5 SUNLinearSolver return codes

The functions provided to SUNLinSol modules by each SUNDIALS package, and functions within the SUNDIALS-provided SUNLinSol implementations, utilize a common set of return codes, listed in Table 8.1. These adhere to a common pattern:

- 0 indicates success
- a positive value corresponds to a recoverable failure, and
- a negative value indicates a non-recoverable failure.

Aside from this pattern, the actual values of each error code provide additional information to the user in case of a linear solver failure.

Table 8.1: SUNLinSol error codes

Error code	Value	Meaning
SUNLS_SUCCESS	0	successful call or converged solve
SUNLS_MEM_NULL	-801	the memory argument to the function is NULL
SUNLS_ILL_INPUT	-802	an illegal input has been provided to the function
SUNLS_MEM_FAIL	-803	failed memory access or allocation
SUNLS_ATIMES_NULL	-804	the ATimes function is NULL
SUNLS_ATIMES_FAIL_UN-REC	-805	an unrecoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_UNREC	-806	an unrecoverable failure occurred in the Pset routine
SUNLS_PSOLVE_NULL	-807	the preconditioner solve function is NULL
SUNLS_PSOLVE_FAIL_UN-REC	-808	an unrecoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_-UNREC	-809	an unrecoverable failure occurred in an external linear solver package
SUNLS_GS_FAIL	-810	a failure occurred during Gram-Schmidt orthogonalization (SPGMR/SPFGMR)
SUNLS_QRSOL_FAIL	-811	a singular R matrix was encountered in a QR factorization (SPGMR/SPFGMR)
SUNLS_VECTOROP_ERR	-812	a vector operation error occurred
SUNLS_RES_REDUCED	801	an iterative solver reduced the residual, but did not converge to the desired tolerance
SUNLS_CONV_FAIL	802	an iterative solver did not converge (and the residual was not reduced)
SUNLS_ATIMES_FAIL_REC	803	a recoverable failure occurred in the ATimes routine
SUNLS_PSET_FAIL_REC	804	a recoverable failure occurred in the Pset routine
SUNLS_PSOLVE_FAIL_REC	805	a recoverable failure occurred in the Psolve routine
SUNLS_PACKAGE_FAIL_-REC	806	a recoverable failure occurred in an external linear solver package
SUNLS_QRFACT_FAIL	807	a singular matrix was encountered during a QR factorization (SPGMR/SPFGMR)
SUNLS_LUFACT_FAIL	808	a singular matrix was encountered during a LU factorization

8.1.6 The generic SUNLinearSolver module

SUNDIALS packages interact with specific SUNLinSol implementations through the generic SUNLinearSolver abstract base class. The `SUNLinearSolver` type is a pointer to a structure containing an implementation-dependent *content* field, and an *ops* field, and is defined as

typedef struct _generic_SUNLinearSolver ***SUNLinearSolver**

and the generic structure is defined as

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

where the `_generic_SUNLinearSolver_Ops` structure is a list of pointers to the various actual linear solver operations provided by a specific implementation. The `_generic_SUNLinearSolver_Ops` structure is defined as

```
struct _generic_SUNLinearSolver_Ops {
  SUNLinearSolver_Type (*gettype)(SUNLinearSolver);
  SUNLinearSolver_ID   (*getid)(SUNLinearSolver);
  int                  (*setatimes)(SUNLinearSolver, void*, SUNATimesFn);
  int                  (*setpreconditioner)(SUNLinearSolver, void*,
                                            SUNPSetupFn, SUNPSolveFn);
  int                  (*setscalingvectors)(SUNLinearSolver,
                                            N_Vector, N_Vector);
  int                  (*setzeroguess)(SUNLinearSolver, booleantype);
  int                  (*initialize)(SUNLinearSolver);
  int                  (*setup)(SUNLinearSolver, SUNMatrix);
  int                  (*solve)(SUNLinearSolver, SUNMatrix, N_Vector,
                                N_Vector, realtype);
  int                  (*numiters)(SUNLinearSolver);
  realtype             (*resnorm)(SUNLinearSolver);
  sunindextype         (*lastflag)(SUNLinearSolver);
  int                  (*space)(SUNLinearSolver, long int*, long int*);
  N_Vector             (*resid)(SUNLinearSolver);
  int                  (*free)(SUNLinearSolver);
};
```

The generic SUNLinSol class defines and implements the linear solver operations defined in §8.1.1 – §8.1.3. These routines are in fact only wrappers to the linear solver operations defined by a particular SUNLinSol implementation, which are accessed through the *ops* field of the `SUNLinearSolver` structure. To illustrate this point we show below the implementation of a typical linear solver operation from the `SUNLinearSolver` base class, namely *SUNLinSolInitialize()*, that initializes a `SUNLinearSolver` object for use after it has been created and configured, and returns a flag denoting a successful or failed operation:

```
int SUNLinSolInitialize(SUNLinearSolver S)
{
  return ((int) S->ops->initialize(S));
}
```

8.1.7 Compatibility of SUNLinearSolver modules

Not all `SUNLinearSolver` implementations are compatible with all `SUNMatrix` and `N_Vector` implementations provided in SUNDIALS. More specifically, all of the SUNDIALS iterative linear solvers (*SPGMR*, *SPFGMR*, *SPBCGS*, *SPTFQMR*, and *PCG*) are compatible with all of the SUNDIALS `N_Vector` modules, but the matrix-based direct SUNLinSol modules are specifically designed to work with distinct `SUNMatrix` and `N_Vector` modules. In the list below, we summarize the compatibility of each matrix-based `SUNLinearSolver` module with the various `SUNMatrix` and `N_Vector` modules. For a more thorough discussion of these compatibilities, we defer to the documentation for each individual SUNLinSol module in the sections that follow.

- *Dense*
    - `SUNMatrix`: *Dense* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *LapackDense*
    - `SUNMatrix`: *Dense* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *Band*
    - `SUNMatrix`: *Band* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *LapackBand*
    - `SUNMatrix`: *Band* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *KLU*
    - `SUNMatrix`: *Sparse* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *SuperLU_MT*
    - `SUNMatrix`: *Sparse* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, or user-supplied
- *SuperLU_Dist*
    - `SUNMatrix`: *SLUNRLOC* or user-supplied
    - `N_Vector`: *Serial*, *OpenMP*, *Pthreads*, *Parallel*, **hypre**, *PETSc*, or user-supplied
- *Magma Dense*
    - `SUNMatrix`: *Magma Dense* or user-supplied
    - `N_Vector`: *HIP*, *RAJA*, or user-supplied
- *OneMKL Dense*
    - `SUNMatrix`: *One MKL Dense* or user-supplied
    - `N_Vector`: *SYCL*, *RAJA*, or user-supplied
- *cuSolverSp batchQR*
    - `SUNMatrix`: *cuSparse* or user-supplied
    - `N_Vector`: *CUDA*, *RAJA*, or user-supplied

8.1.8 Implementing a custom SUNLinearSolver module

A particular implementation of the `SUNLinearSolver` module must:

- Specify the *content* field of the SUNLinSol module.

- Define and implement the required linear solver operations.

Note: The names of these routines should be unique to that implementation in order to permit using more than one SUNLinSol module (each with different `SUNLinearSolver` internal data representations) in the same code.

- Define and implement user-callable constructor and destructor routines to create and free a `SUNLinearSolver` with the new *content* field and with *ops* pointing to the new linear solver operations.

We note that the function pointers for all unsupported optional routines should be set to `NULL` in the *ops* structure. This allows the SUNDIALS package that is using the SUNLinSol object to know whether the associated functionality is supported.

To aid in the creation of custom `SUNLinearSolver` modules the generic `SUNLinearSolver` module provides the utility function *SUNLinSolNewEmpty()*. When used in custom `SUNLinearSolver` constructors this function will ease the introduction of any new optional linear solver operations to the `SUNLinearSolver` API by ensuring that only required operations need to be set.

SUNLinearSolver **SUNLinSolNewEmpty**()

> This function allocates a new generic `SUNLinearSolver` object and initializes its content pointer and the function pointers in the operations structure to `NULL`.
>
> **Return value:**
>
> > If successful, this function returns a `SUNLinearSolver` object. If an error occurs when allocating the object, then this routine will return `NULL`.

void **SUNLinSolFreeEmpty**(*SUNLinearSolver* LS)

> This routine frees the generic `SUNLinearSolver` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is `NULL`, and, if it is not, it will free it as well.
>
> **Arguments:**
>
> - *LS* – a SUNLinearSolver object

Additionally, a `SUNLinearSolver` implementation *may* do the following:

- Define and implement additional user-callable "set" routines acting on the `SUNLinearSolver`, e.g., for setting various configuration options to tune the linear solver for a particular problem.

- Provide additional user-callable "get" routines acting on the `SUNLinearSolver` object, e.g., for returning various solve statistics.

Each SUNLinSol implementation included in SUNDIALS has a unique identifier specified in enumeration and shown in Table 8.2. It is recommended that a user-supplied SUNLinSol implementation use the `SUNLINEARSOLVER_CUSTOM` identifier.

Table 8.2: Identifiers associated with `SUNLinearSolver` modules supplied with SUNDIALS

SUNLinSol ID	Linear solver type	ID Value
SUNLINEARSOLVER_BAND	Banded direct linear solver (internal)	0
SUNLINEARSOLVER_DENSE	Dense direct linear solver (internal)	1
SUNLINEARSOLVER_KLU	Sparse direct linear solver (KLU)	2
SUNLINEARSOLVER_LAPACKBAND	Banded direct linear solver (LAPACK)	3
SUNLINEARSOLVER_LAPACKDENSE	Dense direct linear solver (LAPACK)	4
SUNLINEARSOLVER_PCG	Preconditioned conjugate gradient iterative solver	5
SUNLINEARSOLVER_SPBCGS	Scaled-preconditioned BiCGStab iterative solver	6
SUNLINEARSOLVER_SPFGMR	Scaled-preconditioned FGMRES iterative solver	7
SUNLINEARSOLVER_SPGMR	Scaled-preconditioned GMRES iterative solver	8
SUNLINEARSOLVER_SPTFQMR	Scaled-preconditioned TFQMR iterative solver	9
SUNLINEARSOLVER_SUPERLUDIST	Parallel sparse direct linear solver (SuperLU_Dist)	10
SUNLINEARSOLVER_SUPERLUMT	Threaded sparse direct linear solver (SuperLU_-MT)	11
SUNLINEARSOLVER_CUSOLVERSP_-BATCHQR	Sparse direct linear solver (CUDA)	12
SUNLINEARSOLVER_MAGMADENSE	Dense or block-dense direct linear solver (MAGMA)	13
SUNLINEARSOLVER_ONEMKLDENSE	Dense or block-dense direct linear solver (OneMKL)	14
SUNLINEARSOLVER_CUSTOM	User-provided custom linear solver	15

8.1.8.1 Intended use cases

The SUNLinSol and SUNMATRIX APIs are designed to require a minimal set of routines to ease interfacing with custom or third-party linear solver libraries. Many external solvers provide routines with similar functionality and thus may require minimal effort to wrap within custom SUNMATRIX and SUNLinSol implementations. As SUNDIALS packages utilize generic SUNLinSol modules they may naturally leverage user-supplied `SUNLinearSolver` implementations, thus there exist a wide range of possible linear solver combinations. Some intended use cases for both the SUNDIALS-provided and user-supplied SUNLinSol modules are discussd in the sections below.

Direct linear solvers

Direct linear solver modules require a matrix and compute an "exact" solution to the linear system *defined by the matrix*. SUNDIALS packages strive to amortize the high cost of matrix construction by reusing matrix information for multiple nonlinear iterations or time steps. As a result, each package's linear solver interface recomputes matrix information as infrequently as possible.

Alternative matrix storage formats and compatible linear solvers that are not currently provided by, or interfaced with, SUNDIALS can leverage this infrastructure with minimal effort. To do so, a user must implement custom SUNMA-TRIX and SUNLinSol wrappers for the desired matrix format and/or linear solver following the APIs described in §7 and §8. *This user-supplied SUNLinSol module must then self-identify as having* `SUNLINEARSOLVER_DIRECT` *type*.

Matrix-free iterative linear solvers

Matrix-free iterative linear solver modules do not require a matrix, and instead compute an inexact solution to the linear system *defined by the package-supplied* `ATimes` *routine*. SUNDIALS supplies multiple scaled, preconditioned iterative SUNLinSol modules that support scaling, allowing packages to handle non-dimensionalization, and users to define variables and equations as natural in their applications. However, for linear solvers that do not support left/right scaling, SUNDIALS packages must instead adjust the tolerance supplied to the linear solver to compensate (see the iterative linear tolerance section that follows for more details) – this strategy may be non-optimal since it cannot handle situations where the magnitudes of different solution components or equations vary dramatically within a single application.

To utilize alternative linear solvers that are not currently provided by, or interfaced with, SUNDIALS a user must implement a custom SUNLinSol wrapper for the linear solver following the API described in §8. *This user-supplied SUNLinSol module must then self-identify as having* `SUNLINEARSOLVER_ITERATIVE` *type*.

Matrix-based iterative linear solvers (reusing A)

Matrix-based iterative linear solver modules require a matrix and compute an inexact solution to the linear system *defined by the matrix*. This matrix will be updated infrequently and resued across multiple solves to amortize the cost of matrix construction. As in the direct linear solver case, only thin SUNMATRIX and SUNLinSol wrappers for the underlying matrix and linear solver structures need to be created to utilize such a linear solver. *This user-supplied SUNLinSol module must then self-identify as having* `SUNLINEARSOLVER_MATRIX_ITERATIVE` *type*.

At present, SUNDIALS has one example problem that uses this approach for wrapping a structured-grid matrix, linear solver, and preconditioner from the *hypre* library; this may be used as a template for other customized implementations (see `examples/arkode/CXX_parhyp/ark_heat2D_hypre.cpp`).

Matrix-based iterative linear solvers (current A)

For users who wish to utilize a matrix-based iterative linear solver where the matrix is *purely for preconditioning* and the linear system is *defined by the package-supplied* `ATimes` *routine*, we envision two current possibilities.

The preferred approach is for users to employ one of the SUNDIALS scaled, preconditioned iterative linear solver implementations (*SUNLinSol_SPGMR()*, *SUNLinSol_SPFGMR()*, *SUNLinSol_SPBCGS()*, *SUNLinSol_SPTFQMR()*, or *SUNLinSol_PCG()*) as the outer solver. The creation and storage of the preconditioner matrix, and interfacing with the corresponding matrix-based linear solver, can be handled through a package's preconditioner "setup" and "solve" functionality without creating SUNMATRIX and SUNLinSol implementations. This usage mode is recommended primarily because the SUNDIALS-provided modules support variable and equation scaling as described above.

A second approach supported by the linear solver APIs is as follows. If the SUNLinSol implementation is matrix-based, *self-identifies as having* `SUNLINEARSOLVER_ITERATIVE` *type*, and *also provides a non-NULL SUNLinSolSe-tATimes() routine*, then each SUNDIALS package will call that routine to attach its package-specific matrix-vector product routine to the SUNLinSol object. The SUNDIALS package will then call the SUNLinSol-provided *SUNLin-SolSetup()* routine (infrequently) to update matrix information, but will provide current matrix-vector products to the SUNLinSol implementation through the package-supplied `SUNATimesFn` routine.

Application-specific linear solvers with embedded matrix structure

Many applications can exploit additional linear system structure arising from to the implicit couplings in their model equations. In certain circumstances, the linear solve $Ax = b$ may be performed without the need for a global system matrix A, as the unformed A may be block diagonal or block triangular, and thus the overall linear solve may be performed through a sequence of smaller linear solves. In other circumstances, a linear system solve may be accomplished via specialized fast solvers, such as the fast Fourier transform, fast multipole method, or treecode, in which case no matrix structure may be explicitly necessary. In many of the above situations, construction and preprocessing of the linear system matrix A may be inexpensive, and thus increased performance may be possible if the current linear system information is used within every solve (instead of being lagged, as occurs with matrix-based solvers that reuse A).

To support such application-specific situations, SUNDIALS supports user-provided linear solvers with the `SUNLINEAR-SOLVER_MATRIX_EMBEDDED` type. For an application to leverage this support, it should define a custom SUNLinSol implementation having this type, that only needs to implement the required *SUNLinSolGetType()* and *SUNLinSolSolve()* operations. Within *SUNLinSolSolve()*, the linear solver implementation should call package-specific interface routines (e.g., `ARKStepGetNonlinearSystemData`, `CVodeGetNonlinearSystemData`, `IDAGetNonlinearSystemData`, `ARKStepGetCurrentGamma`, `CVodeGetCurrentGamma`, `IDAGetCurrentCj`, or `MRIStepGetCurrentGamma`) to construct the relevant system matrix A (or portions thereof), solve the linear system $Ax = b$, and return the solution vector x.

We note that when attaching this custom SUNLinearSolver object with the relevant SUNDIALS package `SetLinearSolver` routine, the input *SUNMatrix* `A` should be set to `NULL`.

For templates of such user-provided "matrix-embedded" SUNLinSol implementations, see the SUNDIALS examples `ark_analytic_mels.c`, `cvAnalytic_mels.c`, `cvsAnalytic_mels.c`, `idaAnalytic_mels.c`, and `idasAnalytic_mels.c`.

8.2 CVODE SUNLinearSolver interface

Table 8.3 below lists the `SUNLinearSolver` module linear solver functions used within the CVLS interface. As with the `SUNMatrix` module, we emphasize that the CVODE user does not need to know detailed usage of linear solver functions by the CVODE code modules in order to use CVODE. The information is presented as an implementation detail for the interested reader.

The linear solver functions listed below are marked with 'x' to indicate that they are required, or with † to indicate that they are only called if they are non-`NULL` in the `SUNLinearSolver` implementation that is being used. Note:

1. `SUNLinSolNumIters` is only used to accumulate overall iterative linear solver statistics. If it is not implemented by the `SUNLinearSolver` module, then CVLS will consider all solves as requiring zero iterations.

2. Although CVLS does not call `SUNLinSolLastFlag` directly, this routine is available for users to query linear solver issues directly.

3. Although CVLS does not call `SUNLinSolFree` directly, this routine should be available for users to call when cleaning up from a simulation.

Table 8.3: List of linear solver function usage in the CVLS interface

	DIRECT	ITERATIVE	MATRIX_ITERATIVE
SUNLinSolGetType()	x	x	x
SUNLinSolSetATimes()	†	x	†
SUNLinSolSetPreconditioner()	†	†	†
SUNLinSolSetScalingVectors()	†	†	†
SUNLinSolInitialize()	x	x	x
SUNLinSolSetup()	x	x	x
SUNLinSolSolve()	x	x	x
[1] *SUNLinSolNumIters()*		†	†
[2] *SUNLinSolLastFlag()*			
[3] *SUNLinSolFree()*			
SUNLinSolSpace()	†	†	†

Since there are a wide range of potential `SUNLinearSolver` use cases, the following subsections describe some details of the CVLS interface, in the case that interested users wish to develop custom `SUNLinearSolver` modules.

8.2.1 Lagged matrix information

If the `SUNLinearSolver` object self-identifies as having type `SUNLINEARSOLVER_DIRECT` or `SUNLINEARSOLVER_‐MATRIX_ITERATIVE`, then the `SUNLinearSolver` object solves a linear system *defined* by a `SUNMatrix` object. CVLS will update the matrix information infrequently according to the strategies outlined in §2. To this end, we differentiate between the *desired* linear system $Mx = b$ with $M = (I - \gamma J)$, and the *actual* linear system

$$\bar{M}\bar{x} = b \quad \Leftrightarrow \quad (I - \bar{\gamma}J)\bar{x} = b.$$

Since CVLS updates the `SUNMatrix` object infrequently, it is likely that $\gamma \neq \bar{\gamma}$, and in turn $M \neq \bar{M}$. When using a BDF method, after calling the `SUNLinearSolver`-provided `SUNLinSolSolve` routine, we test whether $\gamma/\bar{\gamma} \neq 1$, and if this is the case we scale the solution $\bar{x}$ to correct the linear system solution x via

$$x = \frac{2}{1 + \gamma/\bar{\gamma}}\bar{x}. \tag{8.3}$$

The motivation for this selection of the scaling factor $c = 2/(1 + \gamma/\bar{\gamma})$ is discussed in detail in [14, 37]. In short, if we consider a stationary iteration for the linear system as consisting of a solve with $\bar{M}$ followed by scaling by c, then for a linear constant-coefficient problem, the error in the solution vector will be reduced at each iteration by the error matrix $E = I - c\bar{M}^{-1}M$, with a convergence rate given by the spectral radius of E. Assuming that stiff systems have a spectrum spread widely over the left half-plane, c is chosen to minimize the magnitude of the eigenvalues of E.

8.2.2 Iterative linear solver tolerance

If the `SUNLinearSolver` object self-identifies as having type `SUNLINEARSOLVER_ITERATIVE` or `SUNLINEAR‐SOLVER_MATRIX_ITERATIVE` then CVLS will set the input tolerance `delta` as described in §2.1. However, if the iterative linear solver does not support scaling matrices (i.e., the `SUNLinSolSetScalingVectors` routine is NULL), then CVLS will attempt to adjust the linear solver tolerance to account for this lack of functionality. To this end, the following assumptions are made:

1. All solution components have similar magnitude; hence the error weight vector W used in the WRMS norm (see §2.1) should satisfy the assumption

$$W_i \approx W_{mean}, \quad \text{for} \quad i = 0, \ldots, n-1.$$

2. The `SUNLinearSolver` object uses a standard 2-norm to measure convergence.

Since CVODE uses identical left and right scaling matrices, $S_1 = S_2 = S = \text{diag}(W)$, then the linear solver convergence requirement is converted as follows (using the notation from equations (8.1) – (8.2)):

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

$$\Leftrightarrow \quad \left\| SP_1^{-1}b - SP_1^{-1}Ax \right\|_2 < \text{tol}$$

$$\Leftrightarrow \quad \sum_{i=0}^{n-1} \left[W_i \left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2$$

$$\Leftrightarrow \quad W_{mean}^2 \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \text{tol}^2$$

$$\Leftrightarrow \quad \sum_{i=0}^{n-1} \left[\left(P_1^{-1}(b - Ax) \right)_i \right]^2 < \left(\frac{\text{tol}}{W_{mean}} \right)^2$$

$$\Leftrightarrow \quad \left\| P_1^{-1}(b - Ax) \right\|_2 < \frac{\text{tol}}{W_{mean}}$$

Therefore the tolerance scaling factor

$$W_{mean} = \|W\|_2 / \sqrt{n}$$

is computed and the scaled tolerance `delta`$= \text{tol}/W_{mean}$ is supplied to the `SUNLinearSolver` object.

8.3 The SUNLinSol_Band Module

The SUNLinSol_Band implementation of the `SUNLinearSolver` class is designed to be used with the corresponding *SUNMATRIX_BAND* matrix type, and one of the serial or shared-memory `N_Vector` implementations (NVECTOR_-SERIAL, NVECTOR_OPENMP or NVECTOR_PTHREADS).

8.3.1 SUNLinSol_Band Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_band.h`. The SUNLinSol_Band module is accessible from all SUNDIALS packages *without* linking to the `libsundials_sunlinsolband` module library.

The SUNLinSol_Band module provides the following user-callable constructor routine:

SUNLinearSolver **SUNLinSol_Band**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

This function creates and allocates memory for a band `SUNLinearSolver`.

Arguments:

- *y* – vector used to determine the linear system size

- *A* – matrix used to assess compatibility

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:
New SUNLinSol_Band object, or `NULL` if either `A` or `y` are incompatible.

Notes:
This routine will perform consistency checks to ensure that it is called with consistent `N_Vector` and `SUNMatrix` implementations. These are currently limited to the SUNMATRIX_BAND matrix type and the

NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

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

For backwards compatibility, we also provide the following wrapper function:

SUNLinearSolver **SUNBandLinearSolver**(*N_Vector* y, *SUNMatrix* A)

Wrapper function for *SUNLinSol_Band()*, with identical input and output arguments.

8.3.2 SUNLinSol_Band Description

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

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

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

- N - size of the linear system,

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

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

This solver is constructed to perform the following operations:

- The "setup" call performs an LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the pivots array.

- The "solve" call performs pivoting and forward and backward substitution using the stored pivots array and the LU factors held in the SUNMATRIX_BAND object.

- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth mu and lower bandwidth ml, then the upper triangular factor U can have upper bandwidth as big as smu = MIN(N-1,mu+ml). The lower triangular factor L has lower bandwidth ml.

The SUNLinSol_Band module defines band implementations of all "direct" linear solver operations listed in §8.1:

- SUNLinSolGetType_Band

- SUNLinSolInitialize_Band – this does nothing, since all consistency checks are performed at solver creation.

- SUNLinSolSetup_Band – this performs the LU factorization.

- SUNLinSolSolve_Band – this uses the LU factors and pivots array to perform the solve.

- SUNLinSolLastFlag_Band

- SUNLinSolSpace_Band – this only returns information for the storage *within* the solver object, i.e. storage for N, last_flag, and pivots.

- SUNLinSolFree_Band

8.4 The SUNLinSol_Dense Module

The SUNLinSol_Dense implementation of the `SUNLinearSolver` class is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory N_Vector implementations (NVECTOR_SERIAL, NVECTOR_OPENMP or NVECTOR_PTHREADS).

8.4.1 SUNLinSol_Dense Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_dense.h`. The SUNLinSol_Dense module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsoldense` module library.

The module SUNLinSol_Dense provides the following user-callable constructor routine:

SUNLinearSolver **SUNLinSol_Dense**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

> This function creates and allocates memory for a dense `SUNLinearSolver`.
>
> **Arguments:**
>
> - *y* – vector used to determine the linear system size.
>
> - *A* – matrix used to assess compatibility.
>
> - *sunctx* – the *SUNContext* object (see §4.1)
>
> **Return value:**
> New SUNLinSol_Dense object, or `NULL` if either `A` or `y` are incompatible.
>
> **Notes:**
> This routine will perform consistency checks to ensure that it is called with consistent `N_Vector` and `SUN-Matrix` implementations. These are currently limited to the SUNMATRIX_DENSE matrix type and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

For backwards compatibility, we also provide the following wrapper function:

SUNLinearSolver **SUNDenseLinearSolver**(*N_Vector* y, *SUNMatrix* A)

> Wrapper function for *SUNLinSol_Dense()*, with identical input and output arguments

8.4.2 SUNLinSol_Dense Description

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

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

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

- `N` - size of the linear system,

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

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

This solver is constructed to perform the following operations:

- The "setup" call performs an LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.

- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

The SUNLinSol_Dense module defines dense implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_Dense`

- `SUNLinSolInitialize_Dense` – this does nothing, since all consistency checks are performed at solver creation.

- `SUNLinSolSetup_Dense` – this performs the LU factorization.

- `SUNLinSolSolve_Dense` – this uses the LU factors and `pivots` array to perform the solve.

- `SUNLinSolLastFlag_Dense`

- `SUNLinSolSpace_Dense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.

- `SUNLinSolFree_Dense`

8.5 The SUNLinSol_KLU Module

The SUNLinSol_KLU implementation of the `SUNLinearSolver` class is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory `N_Vector` implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

8.5.1 SUNLinSol_KLU Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_klu.h`. The installed module library to link to is `libsundials_sunlinsolklu`.*lib* where .*lib* is typically `.so` for shared libraries and `.a` for static libraries.

The module SUNLinSol_KLU provides the following additional user-callable routines:

SUNLinearSolver **SUNLinSol_KLU**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

> This constructor function creates and allocates memory for a SUNLinSol_KLU object.

> **Arguments:**

>> - *y* – vector used to determine the linear system size.

>> - *A* – matrix used to assess compatibility.

>> - *sunctx* – the *SUNContext* object (see §4.1)

> **Return value:**
>> New SUNLinSol_KLU object, or `NULL` if either `A` or `y` are incompatible.

> **Notes:**
>> This routine will perform consistency checks to ensure that it is called with consistent `N_Vector` and SUN-Matrix implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using

either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVEC-TOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

int **SUNLinSol_KLUReInit**(*SUNLinearSolver* S, *SUNMatrix* A, *sunindextype* nnz, int reinit_type)

This function reinitializes memory and flags for a new factorization (symbolic and numeric) to be conducted at the next solver setup call. This routine is useful in the cases where the number of nonzeroes has changed or if the structure of the linear system has changed which would require a new symbolic (and numeric factorization).

Arguments:

- *S* – existing SUNLinSol_KLU object to reinitialize.

- *A* – sparse SUNMatrix matrix (with updated structure) to use for reinitialization.

- *nnz* – maximum number of nonzeros expected for Jacobian matrix.

- *reinit_type* – governs the level of reinitialization. The allowed values are:

    1. The Jacobian matrix will be destroyed and a new one will be allocated based on the nnz value passed to this call. New symbolic and numeric factorizations will be completed at the next solver setup.

    2. Only symbolic and numeric factorizations will be completed. It is assumed that the Jacobian size has not exceeded the size of nnz given in the sparse matrix provided to the original constructor routine (or the previous SUNKLUReInit call).

Return value:

- SUNLS_SUCCESS – reinitialization successful.

- SUNLS_MEM_NULL – either S or A are NULL.

- **SUNLS_ILL_INPUT – A does not have type SUNMATRIX_SPARSE or** reinit_type **is invalid.**

- SUNLS_MEM_FAIL reallocation of the sparse matrix failed.

Notes:

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

int **SUNLinSol_KLUSetOrdering**(*SUNLinearSolver* S, int ordering_choice)

This function sets the ordering used by KLU for reducing fill in the linear solve.

Arguments:

- *S* – existing SUNLinSol_KLU object to update.

- *ordering_choice* – type of ordering to use, options are:

    0. AMD,

    1. COLAMD, and

    2. the natural ordering.

    The default is 1 for COLAMD.

Return value:

- SUNLS_SUCCESS – ordering choice successfully updated.

- SUNLS_MEM_NULL – S is NULL.

- SUNLS_ILL_INPUT – ordering_choice.

sun_klu_symbolic ***SUNLinSol_KLUGetSymbolic**(*SUNLinearSolver* S)

> This function returns a pointer to the KLU symbolic factorization stored in the SUNLinSol_KLU `content` structure.

> When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), sun_klu_symbolic is mapped to the KLU type `klu_symbolic`; when SUNDIALS compiled with 64-bit indices (`SUNDIALS_IN-DEX_SIZE=64`) this is mapped to the KLU type `klu_l_symbolic`.

sun_klu_numeric ***SUNLinSol_KLUGetNumeric**(*SUNLinearSolver* S)

> This function returns a pointer to the KLU numeric factorization stored in the SUNLinSol_KLU `content` structure.

> When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), sun_klu_numeric is mapped to the KLU type `klu_numeric`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_IN-DEX_SIZE=64`) this is mapped to the KLU type `klu_l_numeric`.

sun_klu_common ***SUNLinSol_KLUGetCommon**(*SUNLinearSolver* S)

> This function returns a pointer to the KLU common structure stored in the SUNLinSol_KLU `content` structure.

> When SUNDIALS is compiled with 32-bit indices (`SUNDIALS_INDEX_SIZE=32`), sun_klu_common is mapped to the KLU type `klu_common`; when SUNDIALS is compiled with 64-bit indices (`SUNDIALS_INDEX_SIZE=64`) this is mapped to the KLU type `klu_l_common`.

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNKLU**(*N_Vector* y, *SUNMatrix* A)

> Wrapper function for *SUNLinSol_KLU()*

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

> Wrapper function for *SUNLinSol_KLUReInit()*

int **SUNKLUSetOrdering**(*SUNLinearSolver* S, int ordering_choice)

> Wrapper function for *SUNLinSol_KLUSetOrdering()*

8.5.2 SUNLinSol_KLU Description

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

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

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

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

- `first_factorize` - flag indicating whether the factorization has ever been performed,

- `symbolic` - KLU storage structure for symbolic factorization components, with underlying type `klu_symbolic` or `klu_l_symbolic`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively,

- `numeric` - KLU storage structure for numeric factorization components, with underlying type `klu_numeric` or `klu_l_numeric`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively,

- `common` - storage structure for common KLU solver components, with underlying type `klu_common` or `klu_l_common`, depending on whether SUNDIALS was installed with 32-bit versus 64-bit indices, respectively,

- `klu_solver` – pointer to the appropriate KLU solver function (depending on whether it is using a CSR or CSC sparse matrix, and on whether SUNDIALS was installed with 32-bit or 64-bit indices).

The SUNLinSol_KLU module is a `SUNLinearSolver` wrapper for the KLU sparse matrix factorization and solver library written by Tim Davis and collaborators ([3, 23]). In order to use the SUNLinSol_KLU interface to KLU, it is assumed that KLU has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with KLU (see §11.1.4 for details). Additionally, this wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have *realtype* set to either `extended` or `single` (see *Data Types* for details). Since the KLU library supports both 32-bit and 64-bit integers, this interface will be compiled for either of the available *sunindextype* options.

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

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

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

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.

- On subsequent calls to the "setup" routine, it calls the appropriate KLU "refactor" routine, followed by estimates of the numerical conditioning using the relevant "rcond", and if necessary "condest", routine(s). If these estimates of the condition number are larger than $\varepsilon^{-2/3}$ (where ε is the double-precision unit roundoff), then a new factorization is performed.

- The module includes the routine `SUNKLUReInit`, that can be called by the user to force a full refactorization at the next "setup" call.

- The "solve" call performs pivoting and forward and backward substitution using the stored KLU data structures. We note that in this solve KLU operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The SUNLinSol_KLU module defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_KLU`

- `SUNLinSolInitialize_KLU` – this sets the `first_factorize` flag to 1, forcing both symbolic and numerical factorizations on the subsequent "setup" call.

- `SUNLinSolSetup_KLU` – this performs either a LU factorization or refactorization of the input matrix.

- `SUNLinSolSolve_KLU` – this calls the appropriate KLU solve routine to utilize the LU factors to solve the linear system.

- SUNLinSolLastFlag_KLU

- SUNLinSolSpace_KLU – this only returns information for the storage within the solver *interface*, i.e. storage for the integers last_flag and first_factorize. For additional space requirements, see the KLU documentation.

- SUNLinSolFree_KLU

8.6 The SUNLinSol_LapackBand Module

The SUNLinSol_LapackBand implementation of the SUNLinearSolver class is designed to be used with the corresponding SUNMATRIX_BAND matrix type, and one of the serial or shared-memory N_Vector implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). The

8.6.1 SUNLinSol_LapackBand Usage

The header file to be included when using this module is sunlinsol/sunlinsol_lapackband.h. The installed module library to link to is libsundials_sunlinsollapackband *.lib* where *.lib* is typically .so for shared libraries and .a for static libraries.

The module SUNLinSol_LapackBand provides the following user-callable routine:

SUNLinearSolver **SUNLinSol_LapackBand**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

This function creates and allocates memory for a LAPACK band SUNLinearSolver.

Arguments:

- *y* – vector used to determine the linear system size.

- *A* – matrix used to assess compatibility.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

New SUNLinSol_LapackBand object, or NULL if either A or y are incompatible.

Notes:

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

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

For backwards compatibility, we also provide the following wrapper function:

SUNLinearSolver **SUNLapackBand**(*N_Vector* y, *SUNMatrix* A)

Wrapper function for *SUNLinSol_LapackBand()*, with identical input and output arguments.

8.6.2 SUNLinSol_LapackBand Description

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

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

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

- `N` - size of the linear system,

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

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

The SUNLinSol_LapackBand module is a `SUNLinearSolver` wrapper for the LAPACK band matrix factorization and solve routines, `*GBTRF` and `*GBTRS`, where `*` is either D or S, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see §5.2 for details). In order to use the SUNLinSol_-LapackBand module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see §11.1.4 for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLinSol_LapackBand module also cannot be compiled when using `int64_t` for the `sunindextype`.

This solver is constructed to perform the following operations:

- The "setup" call performs an LU factorization with partial (row) pivoting, $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_BAND object A, with pivoting information encoding P stored in the `pivots` array.

- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_BAND object.

- A must be allocated to accommodate the increase in upper bandwidth that occurs during factorization. More precisely, if A is a band matrix with upper bandwidth `mu` and lower bandwidth `ml`, then the upper triangular factor U can have upper bandwidth as big as `smu = MIN(N-1,mu+ml)`. The lower triangular factor L has lower bandwidth `ml`.

The SUNLinSol_LapackBand module defines band implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_LapackBand`

- `SUNLinSolInitialize_LapackBand` – this does nothing, since all consistency checks are performed at solver creation.

- `SUNLinSolSetup_LapackBand` – this calls either `DGBTRF` or `SGBTRF` to perform the LU factorization.

- `SUNLinSolSolve_LapackBand` – this calls either `DGBTRS` or `SGBTRS` to use the LU factors and `pivots` array to perform the solve.

- `SUNLinSolLastFlag_LapackBand`

- `SUNLinSolSpace_LapackBand` – this only returns information for the storage *within* the solver object, i.e. storage for N, `last_flag`, and `pivots`.

- `SUNLinSolFree_LapackBand`

8.7 The SUNLinSol_LapackDense Module

The SUNLinSol_LapackDense implementation of the `SUNLinearSolver` class is designed to be used with the corresponding SUNMATRIX_DENSE matrix type, and one of the serial or shared-memory `N_Vector` implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS).

8.7.1 SUNLinSol_LapackDense Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_lapackdense.h`. The installed module library to link to is `libsundials_sunlinsollapackdense`.*lib* where *.lib* is typically `.so` for shared libraries and `.a` for static libraries.

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

SUNLinearSolver **SUNLinSol_LapackDense**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

This function creates and allocates memory for a LAPACK dense `SUNLinearSolver`.

Arguments:

- *y* – vector used to determine the linear system size.

- *A* – matrix used to assess compatibility.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

New SUNLinSol_LapackDense object, or `NULL` if either `A` or `y` are incompatible.

Notes:

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

For backwards compatibility, we also provide the following wrapper function:

SUNLinearSolver **SUNLapackDense**(*N_Vector* y, *SUNMatrix* A)

Wrapper function for *SUNLinSol_LapackDense()*, with identical input and output arguments.

8.7.2 SUNLinSol_LapackDense Description

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

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

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

- `N` - size of the linear system,

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

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

The SUNLinSol_LapackDense module is a `SUNLinearSolver` wrapper for the LAPACK dense matrix factorization and solve routines, *GETRF and *GETRS, where * is either D or S, depending on whether SUNDIALS was configured to have `realtype` set to `double` or `single`, respectively (see §5.2 for details). In order to use the SUNLinSol_-LapackDense module it is assumed that LAPACK has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with LAPACK (see §11.1.4 for details). We note that since there do not exist 128-bit floating-point factorization and solve routines in LAPACK, this interface cannot be compiled when using `extended` precision for `realtype`. Similarly, since there do not exist 64-bit integer LAPACK routines, the SUNLinSol_LapackDense module also cannot be compiled when using `int64_t` for the `sunindextype`.

This solver is constructed to perform the following operations:

- The "setup" call performs an LU factorization with partial (row) pivoting ($\mathcal{O}(N^3)$ cost), $PA = LU$, where P is a permutation matrix, L is a lower triangular matrix with 1's on the diagonal, and U is an upper triangular matrix. This factorization is stored in-place on the input SUNMATRIX_DENSE object A, with pivoting information encoding P stored in the `pivots` array.

- The "solve" call performs pivoting and forward and backward substitution using the stored `pivots` array and the LU factors held in the SUNMATRIX_DENSE object ($\mathcal{O}(N^2)$ cost).

The SUNLinSol_LapackDense module defines dense implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_LapackDense`

- `SUNLinSolInitialize_LapackDense` – this does nothing, since all consistency checks are performed at solver creation.

- `SUNLinSolSetup_LapackDense` – this calls either `DGETRF` or `SGETRF` to perform the LU factorization.

- `SUNLinSolSolve_LapackDense` – this calls either `DGETRS` or `SGETRS` to use the LU factors and `pivots` array to perform the solve.

- `SUNLinSolLastFlag_LapackDense`

- `SUNLinSolSpace_LapackDense` – this only returns information for the storage *within* the solver object, i.e. storage for `N`, `last_flag`, and `pivots`.

- `SUNLinSolFree_LapackDense`

8.8 The SUNLinSol_MagmaDense Module

The SUNLinearSolver_MagmaDense implementation of the `SUNLinearSolver` class is designed to be used with the SUNMATRIX_MAGMADENSE matrix, and a GPU-enabled vector. The header file to include when using this module is `sunlinsol/sunlinsol_magmadense.h`. The installed library to link to is `libsundials_-sunlinsolmagmadense.lib` where `lib` is typically `.so` for shared libraries and `.a` for static libraries.

> **Warning:** The SUNLinearSolver_MagmaDense module is experimental and subject to change.

8.8.1 SUNLinearSolver_MagmaDense Description

The SUNLinearSolver_MagmaDense implementation provides an interface to the dense LU and dense batched LU methods in the MAGMA linear algebra library [53]. The batched LU methods are leveraged when solving block diagonal linear systems of the form

$$
\begin{bmatrix}
\mathbf{A_0} & 0 & \cdots & 0 \\
0 & \mathbf{A_1} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \mathbf{A_{n-1}}
\end{bmatrix} x_j = b_j.
$$

8.8.2 SUNLinearSolver_MagmaDense Functions

The SUNLinearSolver_MagmaDense module defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_MagmaDense`

- `SUNLinSolInitialize_MagmaDense`

- `SUNLinSolSetup_MagmaDense`

- `SUNLinSolSolve_MagmaDense`

- `SUNLinSolLastFlag_MagmaDense`

- `SUNLinSolFree_MagmaDense`

In addition, the module provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_MagmaDense**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

> This constructor function creates and allocates memory for a `SUNLinearSolver` object.

> **Arguments:**

> - *y* – a vector for checking compatibility with the solver.

> - *A* – a SUNMATRIX_MAGMADENSE matrix for checking compatibility with the solver.

> - *sunctx* – the *SUNContext* object (see §4.1)

> **Return value:**

> If successful, a `SUNLinearSolver` object. If either *A* or *y* are incompatible then this routine will return NULL. This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the solver.

int **SUNLinSol_MagmaDense_SetAsync**(*SUNLinearSolver* LS, *booleantype* onoff)

> This function can be used to toggle the linear solver between asynchronous and synchronous modes. In asynchronous mode (default), SUNLinearSolver operations are asynchronous with respect to the host. In synchronous mode, the host and GPU device are synchronized prior to the operation returning.

> **Arguments:**

> - *LS* – a SUNLinSol_MagmaDense object

> - *onoff* – 0 for synchronous mode or 1 for asynchronous mode (default 1)

> **Return value:**

> - `SUNLS_SUCCESS` if successful

> - `SUNLS_MEM_NULL` if *LS* is NULL

8.8.3 SUNLinearSolver_MagmaDense Content

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

```
struct _SUNLinearSolverContent_MagmaDense {
  int             last_flag;
  booleantype     async;
  sunindextype    N;
  SUNMemory       pivots;
  SUNMemory       pivotsarr;
  SUNMemory       dpivotsarr;
  SUNMemory       infoarr;
  SUNMemory       rhsarr;
  SUNMemoryHelper memhelp;
  magma_queue_t   q;
};
```

8.9 The SUNLinSol_OneMklDense Module

The SUNLinearSolver_OneMklDense implementation of the `SUNLinearSolver` class interfaces to the direct linear solvers from the Intel oneAPI Math Kernel Library (oneMKL) for solving dense systems or block-diagonal systems with dense blocks. This linear solver is best paired with the SUNMatrix_OneMklDense matrix.

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

> **Warning:** The SUNLinearSolver_OneMklDense class is experimental and subject to change.

8.9.1 SUNLinearSolver_OneMklDense Functions

The SUNLinearSolver_OneMklDense class defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_OneMklDense` – returns `SUNLINEARSOLVER_ONEMKLDENSE`

- `SUNLinSolInitialize_OneMklDense`

- `SUNLinSolSetup_OneMklDense`

- `SUNLinSolSolve_OneMklDense`

- `SUNLinSolLastFlag_OneMklDense`

- `SUNLinSolFree_OneMklDense`

In addition, the class provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_OneMklDense**(*N_Vector* y, *SUNMatrix* A, *SUNContext* sunctx)

   This constructor function creates and allocates memory for a `SUNLinearSolver` object.

   Arguments:

   - *y* – a vector for checking compatibility with the solver.

- *A* – a SUNMatrix_OneMklDense matrix for checking compatibility with the solver.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:
>   If successful, a SUNLinearSolver object. If either *A* or *y* are incompatible then this routine will return NULL. This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the solver.

8.9.2 SUNLinearSolver_OneMklDense Usage Notes

> **Warning:** The SUNLinearSolver_OneMklDense class only supports 64-bit indexing, thus SUNDIALS must be built for 64-bit indexing to use this class.
>
> When using the SUNLinearSolver_OneMklDense class with a SUNDIALS package (e.g. CVODE), the queue given to the matrix is also used for the linear solver.

8.10 The SUNLinSol_PCG Module

The SUNLinSol_PCG implementation of the SUNLinearSolver class performs the PCG (Preconditioned Conjugate Gradient [33]) method; this is an iterative linear solver that is designed to be compatible with any N_Vector implementation that supports a minimal subset of operations (*N_VClone()*, *N_VDotProd()*, *N_VScale()*, *N_VLinearSum()*, *N_VProd()*, and *N_VDestroy()*). Unlike the SPGMR and SPFGMR algorithms, PCG requires a fixed amount of memory that does not increase with the number of allowed iterations.

Unlike all of the other iterative linear solvers supplied with SUNDIALS, PCG should only be used on *symmetric* linear systems (e.g. mass matrix linear systems encountered in ARKODE). As a result, the explanation of the role of scaling and preconditioning matrices given in general must be modified in this scenario. The PCG algorithm solves a linear system $Ax = b$ where A is a symmetric ($A^T = A$), real-valued matrix. Preconditioning is allowed, and is applied in a symmetric fashion on both the right and left. Scaling is also allowed and is applied symmetrically. We denote the preconditioner and scaling matrices as follows:

- P is the preconditioner (assumed symmetric),

- S is a diagonal matrix of scale factors.

The matrices A and P are not required explicitly; only routines that provide A and P^{-1} as operators are required. The diagonal of the matrix S is held in a single N_Vector, supplied by the user.

In this notation, PCG applies the underlying CG algorithm to the equivalent transformed system

$$\tilde{A}\tilde{x} = \tilde{b} \tag{8.4}$$

where

$$
\begin{aligned}
\tilde{A} &= SP^{-1}AP^{-1}S, \\
\tilde{b} &= SP^{-1}b, \\
\tilde{x} &= S^{-1}Px.
\end{aligned}
\tag{8.5}
$$

The scaling matrix must be chosen so that the vectors $SP^{-1}b$ and $S^{-1}Px$ have dimensionless components.

The stopping test for the PCG iterations is on the L2 norm of the scaled preconditioned residual:

$$\|\tilde{b} - \tilde{A}\tilde{x}\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|SP^{-1}b - SP^{-1}Ax\|_2 < \delta$$
$$\Leftrightarrow$$
$$\|P^{-1}b - P^{-1}Ax\|_S < \delta$$

where $\|v\|_S = \sqrt{v^T S^T S v}$, with an input tolerance δ.

8.10.1 SUNLinSol_PCG Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_pcg.h`. The SUNLinSol_PCG module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolpcg` module library.

The module SUNLinSol_PCG provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_PCG**(*N_Vector* y, int pretype, int maxl, *SUNContext* sunctx)

> This constructor function creates and allocates memory for a PCG `SUNLinearSolver`.

> **Arguments:**

> - *y* – a template vector.

> - *pretype* – a flag indicating the type of preconditioning to use:

>   - `SUN_PREC_NONE`

>   - `SUN_PREC_LEFT`

>   - `SUN_PREC_RIGHT`

>   - `SUN_PREC_BOTH`

> - *maxl* – the maximum number of linear iterations to allow.

> - *sunctx* – the *SUNContext* object (see §4.1)

> **Return value:**

> If successful, a `SUNLinearSolver` object. If either *y* is incompatible then this routine will return `NULL`.

> **Notes:**

> This routine will perform consistency checks to ensure that it is called with a consistent `N_Vector` implementation (i.e. that it supplies the requisite vector operations).

> A `maxl` argument that is ≤ 0 will result in the default value (5).

> Since the PCG algorithm is designed to only support symmetric preconditioning, then any of the `pretype` inputs `SUN_PREC_LEFT`, `SUN_PREC_RIGHT`, or `SUN_PREC_BOTH` will result in use of the symmetric preconditioner; any other integer input will result in the default (no preconditioning). Although some SUN-DIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL), PCG should *only* be used with these packages when the linear systems are known to be *symmetric*. Since the scaling of matrix rows and columns must be identical in a symmetric matrix, symmetric preconditioning should work appropriately even for packages designed with one-sided preconditioning in mind.

int **SUNLinSol_PCGSetPrecType**(*SUNLinearSolver* S, int pretype)

> This function updates the flag indicating use of preconditioning.

> **Arguments:**

- *S* – SUNLinSol_PCG object to update.

- *pretype* – a flag indicating the type of preconditioning to use:

    – `SUN_PREC_NONE`

    – `SUN_PREC_LEFT`

    – `SUN_PREC_RIGHT`

    – `SUN_PREC_BOTH`

Return value:

- `SUNLS_SUCCESS` – successful update.

- `SUNLS_ILL_INPUT` – illegal `pretype`

- `SUNLS_MEM_NULL` – S is NULL

Notes:

As above, any one of the input values, `SUN_PREC_LEFT`, `SUN_PREC_RIGHT`, or `SUN_PREC_BOTH` will enable preconditioning; `SUN_PREC_NONE` disables preconditioning.

int **SUNLinSol_PCGSetMaxl**(*SUNLinearSolver* S, int maxl)

This function updates the number of linear solver iterations to allow.

Arguments:

- *S* – SUNLinSol_PCG object to update.

- *maxl* – maximum number of linear iterations to allow. Any non-positive input will result in the default value (5).

Return value:

- `SUNLS_SUCCESS` – successful update.

- `SUNLS_MEM_NULL` – S is NULL

int **SUNLinSolSetInfoFile_PCG**(*SUNLinearSolver* LS, FILE *info_file)

The function *SUNLinSolSetInfoFile_PCG()* sets the output file where all informative (non-error) messages should be directed.

Arguments:

- *LS* – a SUNLinSol object

- *info_file* – **pointer to output file (`stdout` by default);**
    a NULL input will disable output

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

Warning: SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNLinSolSetPrintLevel_PCG**(*SUNLinearSolver* LS, int print_level)

> The function *SUNLinSolSetPrintLevel_PCG()* specifies the level of verbosity of the output.
>
> **Arguments:**
>
> > - *LS* – a SUNLinSol object
> > - *print_level* – flag indicating level of verbosity; must be one of:
> >   - 0, no information is printed (default)
> >   - 1, for each linear iteration the residual norm is printed
>
> **Return value:**
>
> > - *SUNLS_SUCCESS* if successful
> > - *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL
> > - *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled, or if the print level value was invalid
>
> **Notes:**
>
> > This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.
> >
> > **SUNDIALS must be built with the CMake option** `SUNDIALS_BUILD_WITH_MONITORING` **to utilize this function.** See §11.1.2 for more information.
>
> Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNPCG**(*N_Vector* y, int pretype, int maxl)

> Wrapper function for *SUNLinSol_PCG()*

int **SUNPCGSetPrecType**(*SUNLinearSolver* S, int pretype)

> Wrapper function for *SUNLinSol_PCGSetPrecType()*

int **SUNPCGSetMaxl**(*SUNLinearSolver* S, int maxl)

> Wrapper function for *SUNLinSol_PCGSetMaxl()*

8.10.2 SUNLinSol_PCG Description

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

```
struct _SUNLinearSolverContent_PCG {
  int maxl;
  int pretype;
  booleantype zeroguess;
  int numiters;
  realtype resnorm;
  int last_flag;
  SUNATimesFn ATimes;
  void* ATData;
  SUNPSetupFn Psetup;
  SUNPSolveFn Psolve;
```

```
    void* PData;
    N_Vector s;
    N_Vector r;
    N_Vector p;
    N_Vector z;
    N_Vector Ap;
    int     print_level;
    FILE*   info_file;
};
```

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

- maxl - number of PCG iterations to allow (default is 5),

- pretype - flag for use of preconditioning (default is none),

- numiters - number of iterations from the most-recent solve,

- resnorm - final linear residual norm from the most-recent solve,

- last_flag - last error return flag from an internal function,

- ATimes - function pointer to perform Av product,

- ATData - pointer to structure for ATimes,

- Psetup - function pointer to preconditioner setup routine,

- Psolve - function pointer to preconditioner solve routine,

- PData - pointer to structure for Psetup and Psolve,

- s - vector pointer for supplied scaling matrix (default is NULL),

- r - a N_Vector which holds the preconditioned linear system residual,

- p, z, Ap - N_Vector used for workspace by the PCG algorithm.

- print_level - controls the amount of information to be printed to the info file

- info_file - the file where all informative (non-error) messages will be directed

This solver is constructed to perform the following operations:

- During construction all N_Vector solver data is allocated, with vectors cloned from a template N_Vector that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLinSol_PCG to supply the ATimes, PSetup, and Psolve function pointers and s scaling vector.

- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-NULL PSetup function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic PSetup function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call the PCG iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The SUNLinSol_PCG module defines implementations of all "iterative" linear solver operations listed in §8.1:

- SUNLinSolGetType_PCG

- `SUNLinSolInitialize_PCG`

- `SUNLinSolSetATimes_PCG`

- `SUNLinSolSetPreconditioner_PCG`

- `SUNLinSolSetScalingVectors_PCG` – since PCG only supports symmetric scaling, the second `N_Vector` argument to this function is ignored.

- `SUNLinSolSetZeroGuess_PCG` – note the solver assumes a non-zero guess by default and the zero guess flag is reset to `SUNFALSE` after each call to `SUNLinSolSolve_PCG()`.

- `SUNLinSolSetup_PCG`

- `SUNLinSolSolve_PCG`

- `SUNLinSolNumIters_PCG`

- `SUNLinSolResNorm_PCG`

- `SUNLinSolResid_PCG`

- `SUNLinSolLastFlag_PCG`

- `SUNLinSolSpace_PCG`

- `SUNLinSolFree_PCG`

8.11 The SUNLinSol_SPBCGS Module

The SUNLinSol_SPBCGS implementation of the `SUNLinearSolver` class performs a Scaled, Preconditioned, Bi-Conjugate Gradient, Stabilized [56] method; this is an iterative linear solver that is designed to be compatible with any `N_Vector` implementation that supports a minimal subset of operations (*N_VClone()*, *N_VDotProd()*, *N_VScale()*, *N_VLinearSum()*, *N_VProd()*, *N_VDiv()*, and *N_VDestroy()*). Unlike the SPGMR and SPFGMR algorithms, SPBCGS requires a fixed amount of memory that does not increase with the number of allowed iterations.

8.11.1 SUNLinSol_SPBCGS Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_spbcgs.h`. The SUNLinSol_-SPBCGS module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolspbcgs` module library.

The module SUNLinSol_SPBCGS provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_SPBCGS**(*N_Vector* y, int pretype, int maxl, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SPBCGS `SUNLinearSolver`.

Arguments:

- *y* – a template vector.

- *pretype* – a flag indicating the type of preconditioning to use:

  – `SUN_PREC_NONE`

  – `SUN_PREC_LEFT`

  – `SUN_PREC_RIGHT`

  – `SUN_PREC_BOTH`

- *maxl* – the maximum number of linear iterations to allow.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

If successful, a SUNLinearSolver object. If either *y* is incompatible then this routine will return NULL.

Notes:

This routine will perform consistency checks to ensure that it is called with a consistent N_Vector implementation (i.e. that it supplies the requisite vector operations).

A maxl argument that is ≤ 0 will result in the default value (5).

Some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLinSol_SPBCGS object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

Note: With SUN_PREC_RIGHT or SUN_PREC_BOTH the initial guess must be zero (use *SUNLinSolSetZeroGuess()* to indicate the initial guess is zero).

---

int **SUNLinSol_SPBCGSSetPrecType**(*SUNLinearSolver* S, int pretype)

This function updates the flag indicating use of preconditioning.

Arguments:

- *S* – SUNLinSol_SPBCGS object to update.

- *pretype* – a flag indicating the type of preconditioning to use:

    - SUN_PREC_NONE

    - SUN_PREC_LEFT

    - SUN_PREC_RIGHT

    - SUN_PREC_BOTH

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_ILL_INPUT – illegal pretype

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSol_SPBCGSSetMaxl**(*SUNLinearSolver* S, int maxl)

This function updates the number of linear solver iterations to allow.

Arguments:

- *S* – SUNLinSol_SPBCGS object to update.

- *maxl* – maximum number of linear iterations to allow. Any non-positive input will result in the default value (5).

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSolSetInfoFile_SPBCGS**(*SUNLinearSolver* LS, FILE *info_file)

The function *SUNLinSolSetInfoFile_SPBCGS()* sets the output file where all informative (non-error) messages should be directed.

Arguments:

- *LS* – a SUNLinSol object

- *info_file* – **pointer to output file (`stdout` by default);**
  a NULL input will disable output

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

SUNDIALS must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING` **to utilize this function.** See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNLinSolSetPrintLevel_SPBCGS**(*SUNLinearSolver* LS, int print_level)

The function *SUNLinSolSetPrintLevel_SPBCGS()* specifies the level of verbosity of the output.

Arguments:

- *LS* – a SUNLinSol object

- *print_level* – flag indicating level of verbosity; must be one of:

  - 0, no information is printed (default)

  - 1, for each linear iteration the residual norm is printed

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled, or if the print level value was invalid

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

Warning: SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNSPBCGS**(*N_Vector* y, int pretype, int maxl)

Wrapper function for *SUNLinSol_SPBCGS()*

int **SUNSPBCGSSetPrecType**(*SUNLinearSolver* S, int pretype)

Wrapper function for *SUNLinSol_SPBCGSSetPrecType()*

---

int **SUNSPBCGSSetMaxl**(*SUNLinearSolver* S, int maxl)

> Wrapper function for *SUNLinSol_SPBCGSSetMaxl()*

8.11.2 SUNLinSol_SPBCGS Description

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

```
struct _SUNLinearSolverContent_SPBCGS {
  int maxl;
  int pretype;
  booleantype zeroguess;
  int numiters;
  realtype resnorm;
  int last_flag;
  SUNATimesFn ATimes;
  void* ATData;
  SUNPSetupFn Psetup;
  SUNPSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector r;
  N_Vector r_star;
  N_Vector p;
  N_Vector q;
  N_Vector u;
  N_Vector Ap;
  N_Vector vtemp;
  int      print_level;
  FILE*    info_file;
};
```

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

- `maxl` - number of SPBCGS iterations to allow (default is 5),

- `pretype` - flag for type of preconditioning to employ (default is none),

- `numiters` - number of iterations from the most-recent solve,

- `resnorm` - final linear residual norm from the most-recent solve,

- `last_flag` - last error return flag from an internal function,

- `ATimes` - function pointer to perform Av product,

- `ATData` - pointer to structure for `ATimes`,

- `Psetup` - function pointer to preconditioner setup routine,

- `Psolve` - function pointer to preconditioner solve routine,

- `PData` - pointer to structure for `Psetup` and `Psolve`,

- `s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

- `r` - a `N_Vector` which holds the current scaled, preconditioned linear system residual,

- `r_star` - a `N_Vector` which holds the initial scaled, preconditioned linear system residual,

- `p, q, u, Ap, vtemp` - `N_Vector` used for workspace by the SPBCGS algorithm.

- `print_level` - controls the amount of information to be printed to the info file

- `info_file` - the file where all informative (non-error) messages will be directed

This solver is constructed to perform the following operations:

- During construction all `N_Vector` solver data is allocated, with vectors cloned from a template `N_Vector` that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLinSol_SPBCGS to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.

- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call the SPBCGS iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The SUNLinSol_SPBCGS module defines implementations of all "iterative" linear solver operations listed in §8.1:

- SUNLinSolGetType_SPBCGS

- SUNLinSolInitialize_SPBCGS

- SUNLinSolSetATimes_SPBCGS

- SUNLinSolSetPreconditioner_SPBCGS

- SUNLinSolSetScalingVectors_SPBCGS

- SUNLinSolSetZeroGuess_SPBCGS – note the solver assumes a non-zero guess by default and the zero guess flag is reset to SUNFALSE after each call to SUNLinSolSolve_SPBCGS().

- SUNLinSolSetup_SPBCGS

- SUNLinSolSolve_SPBCGS

- SUNLinSolNumIters_SPBCGS

- SUNLinSolResNorm_SPBCGS

- SUNLinSolResid_SPBCGS

- SUNLinSolLastFlag_SPBCGS

- SUNLinSolSpace_SPBCGS

- SUNLinSolFree_SPBCGS

8.12 The SUNLinSol_SPFGMR Module

The SUNLinSol_SPFGMR implementation of the `SUNLinearSolver` class performs a Scaled, Preconditioned, Flexible, Generalized Minimum Residual [49] method; this is an iterative linear solver that is designed to be compatible with any `N_Vector` implementation that supports a minimal subset of operations (`N_VClone()`, `N_VDotProd()`, `N_VScale()`, `N_VLinearSum()`, `N_VProd()`, `N_VConst()`, `N_VDiv()`, and `N_VDestroy()`). Unlike the other Krylov iterative linear solvers supplied with SUNDIALS, FGMRES is specifically designed to work with a changing preconditioner (e.g. from an iterative method).

8.12.1 SUNLinSol_SPFGMR Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_spfgmr.h`. The SUNLinSol_SPFGMR module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolspfgmr` module library.

The module SUNLinSol_SPFGMR provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_SPFGMR**(*N_Vector* y, int pretype, int maxl, *SUNContext* sunctx)

 This constructor function creates and allocates memory for a SPFGMR `SUNLinearSolver`.

 Arguments:

- *y* – a template vector.
- *pretype* – a flag indicating the type of preconditioning to use:
  - SUN_PREC_NONE
  - SUN_PREC_LEFT
  - SUN_PREC_RIGHT
  - SUN_PREC_BOTH
- *maxl* – the number of Krylov basis vectors to use.
- *sunctx* – the *SUNContext* object (see §4.1)

 Return value:

 If successful, a `SUNLinearSolver` object. If either *y* is incompatible then this routine will return `NULL`.

 Notes:

 This routine will perform consistency checks to ensure that it is called with a consistent `N_Vector` implementation (i.e. that it supplies the requisite vector operations).

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

 Since the FGMRES algorithm is designed to only support right preconditioning, then any of the `pretype` inputs SUN_PREC_LEFT, SUN_PREC_RIGHT, or SUN_PREC_BOTH will result in use of SUN_PREC_RIGHT; any other integer input will result in the default (no preconditioning). We note that some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS). While it is possible to use a right-preconditioned SUNLinSol_SPFGMR object for these packages, this use mode is not supported and may result in inferior performance.

int **SUNLinSol_SPFGMRSetPrecType**(*SUNLinearSolver* S, int pretype)

 This function updates the flag indicating use of preconditioning.

 Arguments:

- *S* – SUNLinSol_SPFGMR object to update.

- *pretype* – a flag indicating the type of preconditioning to use:

  - SUN_PREC_NONE

  - SUN_PREC_LEFT

  - SUN_PREC_RIGHT

  - SUN_PREC_BOTH

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_ILL_INPUT – illegal `pretype`

- SUNLS_MEM_NULL – S is NULL

Notes:
   Since the FGMRES algorithm is designed to only support right preconditioning, then any of the `pretype` inputs SUN_PREC_LEFT, SUN_PREC_RIGHT, or SUN_PREC_BOTH will result in use of SUN_PREC_RIGHT; any other integer input will result in the default (no preconditioning).

int **SUNLinSol_SPFGMRSetGSType**(*SUNLinearSolver* S, int gstype)

This function sets the type of Gram-Schmidt orthogonalization to use.

Arguments:

- *S* – SUNLinSol_SPFGMR object to update.

- *gstype* – a flag indicating the type of orthogonalization to use:

  - SUN_MODIFIED_GS

  - SUN_CLASSICAL_GS

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_ILL_INPUT – illegal `gstype`

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSol_SPFGMRSetMaxRestarts**(*SUNLinearSolver* S, int maxrs)

This function sets the number of FGMRES restarts to allow.

Arguments:

- *S* – SUNLinSol_SPFGMR object to update.

- *maxrs* – maximum number of restarts to allow. A negative input will result in the default of 0.

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSolSetInfoFile_SPFGMR**(*SUNLinearSolver* LS, FILE *info_file)

The function *SUNLinSolSetInfoFile_SPFGMR()* sets the output file where all informative (non-error) messages should be directed.

Arguments:

- *LS* – a SUNLinSol object

- *info_file* – **pointer to output file (`stdout` by default)**;
    a NULL input will disable output

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

Warning: SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNLinSolSetPrintLevel_SPFGMR**(*SUNLinearSolver* LS, int print_level)

The function *SUNLinSolSetPrintLevel_SPFGMR()* specifies the level of verbosity of the output.

Arguments:

- *LS* – a SUNLinSol object

- *print_level* – flag indicating level of verbosity; must be one of:

    - 0, no information is printed (default)

    - 1, for each linear iteration the residual norm is printed

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled, or if the print level value was invalid

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNSPFGMR**(*N_Vector* y, int pretype, int maxl)

Wrapper function for *SUNLinSol_SPFGMR()*

int **SUNSPFGMRSetPrecType**(*SUNLinearSolver* S, int pretype)

Wrapper function for *SUNLinSol_SPFGMRSetPrecType()*

int **SUNSPFGMRSetGSType**(*SUNLinearSolver* S, int gstype)

Wrapper function for *SUNLinSol_SPFGMRSetGSType()*

---

int **SUNSPFGMRSetMaxRestarts**(*SUNLinearSolver* S, int maxrs)

      Wrapper function for *SUNLinSol_SPFGMRSetMaxRestarts()*

8.12.2 SUNLinSol_SPFGMR Description

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

```
struct _SUNLinearSolverContent_SPFGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  booleantype zeroguess;
  int numiters;
  realtype resnorm;
  int last_flag;
  SUNATimesFn ATimes;
  void* ATData;
  SUNPSetupFn Psetup;
  SUNPSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector *V;
  N_Vector *Z;
  realtype **Hes;
  realtype *givens;
  N_Vector xcor;
  realtype *yg;
  N_Vector vtemp;
  int     print_level;
  FILE*   info_file;
};
```

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

- `maxl` - number of FGMRES basis vectors to use (default is 5),

- `pretype` - flag for use of preconditioning (default is none),

- `gstype` - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

- `max_restarts` - number of FGMRES restarts to allow (default is 0),

- `numiters` - number of iterations from the most-recent solve,

- `resnorm` - final linear residual norm from the most-recent solve,

- `last_flag` - last error return flag from an internal function,

- `ATimes` - function pointer to perform Av product,

- `ATData` - pointer to structure for `ATimes`,

- `Psetup` - function pointer to preconditioner setup routine,

- `Psolve` - function pointer to preconditioner solve routine,

- `PData` - pointer to structure for `Psetup` and `Psolve`,

- `s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

- `V` - the array of Krylov basis vectors $v_1, \ldots, v_{\text{maxl}+1}$, stored in `V[0], ..., V[maxl]`. Each v_i is a vector of type `N_Vector`,

- `Z` - the array of preconditioned Krylov basis vectors $z_1, \ldots, z_{\text{maxl}+1}$, stored in `Z[0], ..., Z[maxl]`. Each z_i is a vector of type `N_Vector`,

- `Hes` - the $(\text{maxl} + 1) \times \text{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`,

- `givens` - a length $2\,\text{maxl}$ array which represents the Givens rotation matrices that arise in the FGMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where

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

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

- `xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

- `yg` - a length $(\text{maxl} + 1)$ array of `realtype` values used to hold "short" vectors (e.g. y and g),

- `vtemp` - temporary vector storage.

- `print_level` - controls the amount of information to be printed to the info file

- `info_file` - the file where all informative (non-error) messages will be directed

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template `N_Vector` that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLinSol_SPFGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.

- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)

- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call, the FGMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

The SUNLinSol_SPFGMR module defines implementations of all "iterative" linear solver operations listed in §8.1:

- `SUNLinSolGetType_SPFGMR`

- `SUNLinSolInitialize_SPFGMR`

- `SUNLinSolSetATimes_SPFGMR`

- `SUNLinSolSetPreconditioner_SPFGMR`

- `SUNLinSolSetScalingVectors_SPFGMR`

- `SUNLinSolSetZeroGuess_SPFGMR` – note the solver assumes a non-zero guess by default and the zero guess flag is reset to `SUNFALSE` after each call to `SUNLinSolSolve_SPFGMR()`.

- `SUNLinSolSetup_SPFGMR`

- `SUNLinSolSolve_SPFGMR`

- `SUNLinSolNumIters_SPFGMR`

- `SUNLinSolResNorm_SPFGMR`

- `SUNLinSolResid_SPFGMR`

- `SUNLinSolLastFlag_SPFGMR`

- `SUNLinSolSpace_SPFGMR`

- `SUNLinSolFree_SPFGMR`

8.13 The SUNLinSol_SPGMR Module

The SUNLinSol_SPGMR implementation of the `SUNLinearSolver` class performs a Scaled, Preconditioned, Generalized Minimum Residual [50] method; this is an iterative linear solver that is designed to be compatible with any `N_Vector` implementation that supports a minimal subset of operations (`N_VClone()`, `N_VDotProd()`, `N_VScale()`, `N_VLinearSum()`, `N_VProd()`, `N_VConst()`, `N_VDiv()`, and `N_VDestroy()`).

8.13.1 SUNLinSol_SPGMR Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_spgmr.h`. The SUNinSol_SPGMR module is accessible from all SUNDIALS solvers *without* linking to the `libsundials_sunlinsolspgmr` module library.

The module SUNLinSol_SPGMR provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_SPGMR**(*N_Vector* y, int pretype, int maxl, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SPGMR `SUNLinearSolver`.

Arguments:

- *y* – a template vector.

- *pretype* – a flag indicating the type of preconditioning to use:

    – `SUN_PREC_NONE`

    – `SUN_PREC_LEFT`

    – `SUN_PREC_RIGHT`

    – `SUN_PREC_BOTH`

- *maxl* – the number of Krylov basis vectors to use.

Return value:

If successful, a `SUNLinearSolver` object. If either *y* is incompatible then this routine will return `NULL`.

Notes:

This routine will perform consistency checks to ensure that it is called with a consistent `N_Vector` implementation (i.e. that it supplies the requisite vector operations).

A maxl argument that is ≤ 0 will result in the default value (5).

Some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLinSol_SPGMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

int **SUNLinSol_SPGMRSetPrecType**(*SUNLinearSolver* S, int pretype)

This function updates the flag indicating use of preconditioning.

Arguments:

- *S* – SUNLinSol_SPGMR object to update.

- *pretype* – a flag indicating the type of preconditioning to use:

    – SUN_PREC_NONE

    – SUN_PREC_LEFT

    – SUN_PREC_RIGHT

    – SUN_PREC_BOTH

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_ILL_INPUT – illegal pretype

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSol_SPGMRSetGSType**(*SUNLinearSolver* S, int gstype)

This function sets the type of Gram-Schmidt orthogonalization to use.

Arguments:

- *S* – SUNLinSol_SPGMR object to update.

- *gstype* – a flag indicating the type of orthogonalization to use:

    – SUN_MODIFIED_GS

    – SUN_CLASSICAL_GS

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_ILL_INPUT – illegal gstype

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSol_SPGMRSetMaxRestarts**(*SUNLinearSolver* S, int maxrs)

This function sets the number of GMRES restarts to allow.

Arguments:

- *S* – SUNLinSol_SPGMR object to update.

- *maxrs* – maximum number of restarts to allow. A negative input will result in the default of 0.

Return value:

- SUNLS_SUCCESS – successful update.

- SUNLS_MEM_NULL – S is NULL

int **SUNLinSolSetInfoFile_SPGMR**(*SUNLinearSolver* LS, FILE *info_file)

The function *SUNLinSolSetInfoFile_SPGMR()* sets the output file where all informative (non-error) messages should be directed.

Arguments:

- *LS* – a SUNLinSol object

- *info_file* – pointer to output file (`stdout` by default); a `NULL` input will disable output

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was `NULL`

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

> **Warning:** SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNLinSolSetPrintLevel_SPGMR**(*SUNLinearSolver* LS, int print_level)

The function *SUNLinSolSetPrintLevel_SPGMR()* specifies the level of verbosity of the output.

Arguments:

- *LS* – a SUNLinSol object

- *print_level* – flag indicating level of verbosity; must be one of:

    - 0, no information is printed (default)

    - 1, for each linear iteration the residual norm is printed

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was `NULL`

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled, or if the print level value was invalid

Notes:

This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING` **to utilize this function.** See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

For backwards compatibility, we also provide the wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNSPGMR**(*N_Vector* y, int pretype, int maxl)

Wrapper function for *SUNLinSol_SPGMR()*

int **SUNSPGMRSetPrecType**(*SUNLinearSolver* S, int pretype)

>   Wrapper function for *SUNLinSol_SPGMRSetPrecType()*

int **SUNSPGMRSetGSType**(*SUNLinearSolver* S, int gstype)

>   Wrapper function for *SUNLinSol_SPGMRSetGSType()*

int **SUNSPGMRSetMaxRestarts**(*SUNLinearSolver* S, int maxrs)

>   Wrapper function for *SUNLinSol_SPGMRSetMaxRestarts()*

8.13.2 SUNLinSol_SPGMR Description

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

```
struct _SUNLinearSolverContent_SPGMR {
  int maxl;
  int pretype;
  int gstype;
  int max_restarts;
  booleantype zeroguess;
  int numiters;
  realtype resnorm;
  int last_flag;
  SUNATimesFn ATimes;
  void* ATData;
  SUNPSetupFn Psetup;
  SUNPSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector *V;
  realtype **Hes;
  realtype *givens;
  N_Vector xcor;
  realtype *yg;
  N_Vector vtemp;
  int      print_level;
  FILE*    info_file;
};
```

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

- maxl - number of GMRES basis vectors to use (default is 5),

- pretype - flag for type of preconditioning to employ (default is none),

- gstype - flag for type of Gram-Schmidt orthogonalization (default is modified Gram-Schmidt),

- max_restarts - number of GMRES restarts to allow (default is 0),

- numiters - number of iterations from the most-recent solve,

- resnorm - final linear residual norm from the most-recent solve,

- last_flag - last error return flag from an internal function,

- ATimes - function pointer to perform Av product,

- ATData - pointer to structure for ATimes,

- `Psetup` - function pointer to preconditioner setup routine,

- `Psolve` - function pointer to preconditioner solve routine,

- `PData` - pointer to structure for `Psetup` and `Psolve`,

- `s1, s2` - vector pointers for supplied scaling matrices (default is `NULL`),

- `V` - the array of Krylov basis vectors $v_1, \ldots, v_{\mathrm{maxl}+1}$, stored in `V[0], ... V[maxl]`. Each v_i is a vector of type `N_Vector`,

- `Hes` - the $(\mathrm{maxl} + 1) \times \mathrm{maxl}$ Hessenberg matrix. It is stored row-wise so that the (i,j)th element is given by `Hes[i][j]`,

- `givens` - a length $2\,\mathrm{maxl}$ array which represents the Givens rotation matrices that arise in the GMRES algorithm. These matrices are $F_0, F_1, \ldots, F_j$, where

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

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

- `xcor` - a vector which holds the scaled, preconditioned correction to the initial guess,

- `yg` - a length $(\mathrm{maxl} + 1)$ array of `realtype` values used to hold "short" vectors (e.g. y and g),

- `vtemp` - temporary vector storage.

- `print_level` - controls the amount of information to be printed to the info file

- `info_file` - the file where all informative (non-error) messages will be directed

This solver is constructed to perform the following operations:

- During construction, the `xcor` and `vtemp` arrays are cloned from a template `N_Vector` that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLinSol_SPGMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.

- In the "initialize" call, the remaining solver data is allocated (`V`, `Hes`, `givens`, and `yg`)

- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call, the GMRES iteration is performed. This will include scaling, preconditioning, and restarts if those options have been supplied.

The SUNLinSol_SPGMR module defines implementations of all "iterative" linear solver operations listed in §8.1:

- `SUNLinSolGetType_SPGMR`

- `SUNLinSolInitialize_SPGMR`

- SUNLinSolSetATimes_SPGMR

- SUNLinSolSetPreconditioner_SPGMR

- SUNLinSolSetScalingVectors_SPGMR

- SUNLinSolSetZeroGuess_SPGMR – note the solver assumes a non-zero guess by default and the zero guess flag is reset to SUNFALSE after each call to SUNLinSolSolve_SPGMR().

- SUNLinSolSetup_SPGMR

- SUNLinSolSolve_SPGMR

- SUNLinSolNumIters_SPGMR

- SUNLinSolResNorm_SPGMR

- SUNLinSolResid_SPGMR

- SUNLinSolLastFlag_SPGMR

- SUNLinSolSpace_SPGMR

- SUNLinSolFree_SPGMR

8.14 The SUNLinSol_SPTFQMR Module

The SUNLinSol_SPTFQMR implementation of the SUNLinearSolver class performs a Scaled, Preconditioned, Transpose-Free Quasi-Minimum Residual [31] method; this is an iterative linear solver that is designed to be compatible with any N_Vector implementation that supports a minimal subset of operations (*N_VClone()*, *N_VDotProd()*, *N_VScale()*, *N_VLinearSum()*, *N_VProd()*, *N_VConst()*, *N_VDiv()*, and *N_VDestroy()*). Unlike the SPGMR and SPFGMR algorithms, SPTFQMR requires a fixed amount of memory that does not increase with the number of allowed iterations.

8.14.1 SUNLinSol_SPTFQMR Usage

The header file to be included when using this module is sunlinsol/sunlinsol_sptfqmr.h. The SUNLinSol_SPT-FQMR module is accessible from all SUNDIALS solvers *without* linking to the libsundials_sunlinsolsptfqmr module library.

The module SUNLinSol_SPTFQMR provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_SPTFQMR**(*N_Vector* y, int pretype, int maxl, *SUNContext* sunctx)

    This constructor function creates and allocates memory for a SPTFQMR SUNLinearSolver.

    Arguments:

- *y* – a template vector.

- *pretype* – a flag indicating the type of preconditioning to use:
    - SUN_PREC_NONE
    - SUN_PREC_LEFT
    - SUN_PREC_RIGHT
    - SUN_PREC_BOTH

- *maxl* – the number of Krylov basis vectors to use.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

      If successful, a SUNLinearSolver object. If either *y* is incompatible then this routine will return NULL.

Notes:

      This routine will perform consistency checks to ensure that it is called with a consistent N_Vector implementation (i.e. that it supplies the requisite vector operations).

      A maxl argument that is ≤ 0 will result in the default value (5).

      Some SUNDIALS solvers are designed to only work with left preconditioning (IDA and IDAS) and others with only right preconditioning (KINSOL). While it is possible to configure a SUNLinSol_SPTFQMR object to use any of the preconditioning options with these solvers, this use mode is not supported and may result in inferior performance.

Note: With SUN_PREC_RIGHT or SUN_PREC_BOTH the initial guess must be zero (use *SUNLinSolSetZeroGuess()* to indicate the initial guess is zero).

---

int **SUNLinSol_SPTFQMRSetPrecType**(*SUNLinearSolver* S, int pretype)

This function updates the flag indicating use of preconditioning.

Arguments:

- *S* – SUNLinSol_SPGMR object to update.
- *pretype* – a flag indicating the type of preconditioning to use:
    - SUN_PREC_NONE
    - SUN_PREC_LEFT
    - SUN_PREC_RIGHT
    - SUN_PREC_BOTH

Return value:

- SUNLS_SUCCESS – successful update.
- SUNLS_ILL_INPUT – illegal pretype
- SUNLS_MEM_NULL – S is NULL

int **SUNLinSol_SPTFQMRSetMaxl**(*SUNLinearSolver* S, int maxl)

This function updates the number of linear solver iterations to allow.

Arguments:

- *S* – SUNLinSol_SPTFQMR object to update.
- *maxl* – maximum number of linear iterations to allow. Any non-positive input will result in the default value (5).

Return value:

- SUNLS_SUCCESS – successful update.
- SUNLS_MEM_NULL – S is NULL

int **SUNLinSolSetInfoFile_SPTFQMR**(*SUNLinearSolver* LS, FILE *info_file)

The function *SUNLinSolSetInfoFile_SPTFQMR()* sets the output file where all informative (non-error) messages should be directed.

Arguments:

- *LS* – a SUNLinSol object

- *info_file* – **pointer to output file (`stdout` by default);**
    a NULL input will disable output

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled

Notes:
This function is intended for users that wish to monitor the linear solver progress. By default, the file pointer is set to `stdout`.

Warning: SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNLinSolSetPrintLevel_SPTFQMR**(*SUNLinearSolver* LS, int print_level)

The function *SUNLinSolSetPrintLevel_SPTFQMR()* specifies the level of verbosity of the output.

Arguments:

- *LS* – a SUNLinSol object

- *print_level* – flag indicating level of verbosity; must be one of:

    – 0, no information is printed (default)

    – 1, for each linear iteration the residual norm is printed

Return value:

- *SUNLS_SUCCESS* if successful

- *SUNLS_MEM_NULL* if the SUNLinearSolver memory was NULL

- *SUNLS_ILL_INPUT* if SUNDIALS was not built with monitoring enabled, or if the print level value was invalid

Notes:
This function is intended for users that wish to monitor the linear solver progress. By default, the print level is 0.

SUNDIALS must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNSPTFQMR**(*N_Vector* y, int pretype, int maxl)

Wrapper function for *SUNLinSol_SPTFQMR()*

int **SUNSPTFQMRSetPrecType**(*SUNLinearSolver* S, int pretype)

Wrapper function for *SUNLinSol_SPTFQMRSetPrecType()*

int **SUNSPTFQMRSetMaxl**(*SUNLinearSolver* S, int maxl)

      Wrapper function for *SUNLinSol_SPTFQMRSetMaxl()*

8.14.2 SUNLinSol_SPTFQMR Description

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

```
struct _SUNLinearSolverContent_SPTFQMR {
  int maxl;
  int pretype;
  booleantype zeroguess;
  int numiters;
  realtype resnorm;
  int last_flag;
  SUNATimesFn ATimes;
  void* ATData;
  SUNPSetupFn Psetup;
  SUNPSolveFn Psolve;
  void* PData;
  N_Vector s1;
  N_Vector s2;
  N_Vector r_star;
  N_Vector q;
  N_Vector d;
  N_Vector v;
  N_Vector p;
  N_Vector *r;
  N_Vector u;
  N_Vector vtemp1;
  N_Vector vtemp2;
  N_Vector vtemp3;
  int      print_level;
  FILE*    info_file;
};
```

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

- `maxl` - number of TFQMR iterations to allow (default is 5),

- `pretype` - flag for type of preconditioning to employ (default is none),

- `numiters` - number of iterations from the most-recent solve,

- `resnorm` - final linear residual norm from the most-recent solve,

- `last_flag` - last error return flag from an internal function,

- `ATimes` - function pointer to perform Av product,

- `ATData` - pointer to structure for `ATimes`,

- `Psetup` - function pointer to preconditioner setup routine,

- `Psolve` - function pointer to preconditioner solve routine,

- `PData` - pointer to structure for `Psetup` and `Psolve`,

- `s1, s2` - vector pointers for supplied scaling matrices (default is NULL),

- `r_star` - a `N_Vector` which holds the initial scaled, preconditioned linear system residual,

- `q, d, v, p, u` - `N_Vector` used for workspace by the SPTFQMR algorithm,

- `r` - array of two `N_Vector` used for workspace within the SPTFQMR algorithm,

- `vtemp1, vtemp2, vtemp3` - temporary vector storage.

- `print_level` - controls the amount of information to be printed to the info file

- `info_file` - the file where all informative (non-error) messages will be directed

This solver is constructed to perform the following operations:

- During construction all `N_Vector` solver data is allocated, with vectors cloned from a template `N_Vector` that is input, and default solver parameters are set.

- User-facing "set" routines may be called to modify default solver parameters.

- Additional "set" routines are called by the SUNDIALS solver that interfaces with SUNLinSol_SPTFQMR to supply the `ATimes`, `PSetup`, and `Psolve` function pointers and `s1` and `s2` scaling vectors.

- In the "initialize" call, the solver parameters are checked for validity.

- In the "setup" call, any non-`NULL` `PSetup` function is called. Typically, this is provided by the SUNDIALS solver itself, that translates between the generic `PSetup` function and the solver-specific routine (solver-supplied or user-supplied).

- In the "solve" call the TFQMR iteration is performed. This will include scaling and preconditioning if those options have been supplied.

The SUNLinSol_SPTFQMR module defines implementations of all "iterative" linear solver operations listed in §8.1:

- `SUNLinSolGetType_SPTFQMR`

- `SUNLinSolInitialize_SPTFQMR`

- `SUNLinSolSetATimes_SPTFQMR`

- `SUNLinSolSetPreconditioner_SPTFQMR`

- `SUNLinSolSetScalingVectors_SPTFQMR`

- `SUNLinSolSetZeroGuess_SPTFQMR` – note the solver assumes a non-zero guess by default and the zero guess flag is reset to `SUNFALSE` after each call to `SUNLinSolSolve_SPTFQMR()`.

- `SUNLinSolSetup_SPTFQMR`

- `SUNLinSolSolve_SPTFQMR`

- `SUNLinSolNumIters_SPTFQMR`

- `SUNLinSolResNorm_SPTFQMR`

- `SUNLinSolResid_SPTFQMR`

- `SUNLinSolLastFlag_SPTFQMR`

- `SUNLinSolSpace_SPTFQMR`

- `SUNLinSolFree_SPTFQMR`

8.15 The SUNLinSol_SuperLUDIST Module

The SUNLinsol_SuperLUDIST implementation of the `SUNLinearSolver` class interfaces with the SuperLU_DIST library. This is designed to be used with the SUNMatrix_SLUNRloc *SUNMatrix*, and one of the serial, threaded or parallel N_Vector implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, NVECTOR_PTHREADS, NVECTOR_PARALLEL, NVECTOR_PARHYP).

8.15.1 SUNLinSol_SuperLUDIST Usage

The header file to be included when using this module is `sunlinsol/sunlinsol_superludist.h`. The installed module library to link to is `libsundials_sunlinsolsuperludist`.*lib* where *lib* is typically `.so` for shared libraries and `.a` for static libraries.

The module SUNLinSol_SuperLUDIST provides the following user-callable routines:

> **Warning:** Starting with SuperLU_DIST version 6.3.0, some structures were renamed to have a prefix for the floating point type. The double precision API functions have the prefix 'd'. To maintain backwards compatibility with the unprefixed types, SUNDIALS provides macros to these SuperLU_DIST types with an 'x' prefix that expand to the correct prefix. E.g., the SUNDIALS macro `xLUstruct_t` expands to `dLUstruct_t` or `LUstruct_t` based on the SuperLU_DIST version.

SUNLinearSolver **SUNLinSol_SuperLUDIST**(*N_Vector* y, SuperMatrix *A, gridinfo_t *grid, xLUstruct_t *lu, xScalePermstruct_t *scaleperm, xSOLVEstruct_t *solve, SuperLUStat_t *stat, superlu_dist_options_t *options, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SUNLinSol_SuperLUDIST object.

Arguments:

- *y* – a template vector.

- *A* – a template matrix

- *grid*, *lu*, *scaleperm*, *solve*, *stat*, *options* – SuperLU_DIST object pointers.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

If successful, a `SUNLinearSolver` object; otherwise this routine will return NULL.

Notes:

This routine analyzes the input matrix and vector to determine the linear system size and to assess the compatibility with the SuperLU_DIST library.

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

The `grid`, `lu`, `scaleperm`, `solve`, and `options` arguments are not checked and are passed directly to SuperLU_DIST routines.

Some struct members of the `options` argument are modified internally by the SUNLinSol_SuperLUDIST solver. Specifically, the member `Fact` is modified in the setup and solve routines.

realtype **SUNLinSol_SuperLUDIST_GetBerr**(*SUNLinearSolver* LS)

> This function returns the componentwise relative backward error of the computed solution. It takes one argument, the SUNLinearSolver object. The return type is `realtype`.

gridinfo_t ***SUNLinSol_SuperLUDIST_GetGridinfo**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that contains the 2D process grid. It takes one argument, the SUNLinearSolver object.

xLUstruct_t ***SUNLinSol_SuperLUDIST_GetLUstruct**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that contains the distributed L and U structures. It takes one argument, the SUNLinearSolver object.

superlu_dist_options_t ***SUNLinSol_SuperLUDIST_GetSuperLUOptions**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that contains the options which control how the linear system is factorized and solved. It takes one argument, the SUNLinearSolver object.

xScalePermstruct_t ***SUNLinSol_SuperLUDIST_GetScalePermstruct**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that contains the vectors that describe the transformations done to the matrix A. It takes one argument, the SUNLinearSolver object.

xSOLVEstruct_t ***SUNLinSol_SuperLUDIST_GetSOLVEstruct**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that contains information for communication during the solution phase. It takes one argument the SUNLinearSolver object.

SuperLUStat_t ***SUNLinSol_SuperLUDIST_GetSuperLUStat**(*SUNLinearSolver* LS)

> This function returns a pointer to the SuperLU_DIST structure that stores information about runtime and flop count. It takes one argument, the SUNLinearSolver object.

8.15.2 SUNLinSol_SuperLUDIST Description

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

```
struct _SUNLinearSolverContent_SuperLUDIST {
  booleantype          first_factorize;
  int                  last_flag;
  realtype             berr;
  gridinfo_t           *grid;
  xLUstruct_t          *lu;
  superlu_dist_options_t  *options;
  xScalePermstruct_t   *scaleperm;
  xSOLVEstruct_t       *solve;
  SuperLUStat_t        *stat;
  sunindextype         N;
};
```

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

- `first_factorize` – flag indicating whether the factorization has ever been performed,

- `last_flag` – last error return flag from internal function evaluations,

- `berr` – the componentwise relative backward error of the computed solution,

- `grid` – pointer to the SuperLU_DIST structure that strores the 2D process grid

- `lu` – pointer to the SuperLU_DIST structure that stores the distributed L and U factors,

- `scaleperm` – pointer to the SuperLU_DIST structure that stores vectors describing the transformations done to the matrix `A`,

- `options` – pointer to the SuperLU_DIST stucture which contains options that control how the linear system is factorized and solved,

- `solve` – pointer to the SuperLU_DIST solve structure,

- `stat` – pointer to the SuperLU_DIST structure that stores information about runtime and flop count,

- `N` – the number of equations in the system.

The SUNLinSol_SuperLUDIST module is a SUNLinearSolver adapter for the SuperLU_DIST sparse matrix factorization and solver library written by X. Sherry Li and collaborators [7, 32, 45, 46]. The package uses a SPMD parallel programming model and multithreading to enhance efficiency in distributed-memory parallel environments with multicore nodes and possibly GPU accelerators. It uses MPI for communication, OpenMP for threading, and CUDA for GPU support. In order to use the SUNLinSol_SuperLUDIST interface to SuperLU_DIST, it is assumed that SuperLU_DIST has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SuperLU_DIST (see §11.1.4 for details). Additionally, the wrapper only supports double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to use single or extended precision. Moreover, since the SuperLU_DIST library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SuperLU_DIST library is installed using the same integer size as SUNDIALS.

The SuperLU_DIST library provides many options to control how a linear system will be factorized and solved. These options may be set by a user on an instance of the `superlu_dist_options_t` struct, and then it may be provided as an argument to the SUNLinSol_SuperLUDIST constructor. The SUNLinSol_SuperLUDIST module will respect all options set except for `Fact` – this option is necessarily modified by the SUNLinSol_SuperLUDIST module in the setup and solve routines.

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

- The first time that the "setup" routine is called, it sets the SuperLU_DIST option `Fact` to `DOFACT` so that a subsequent call to the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to solve the system.

- On subsequent calls to the "setup" routine, it sets the SuperLU_DIST option `Fact` to `SamePattern` so that a subsequent call to "solve" will perform factorization assuming the same sparsity pattern as prior, i.e. it will reuse the column permutation vector.

- If "setup" is called prior to the "solve" routine, then the "solve" routine will perform a symbolic factorization, followed by an initial numerical factorization before continuing to the sparse triangular solves, and, potentially, iterative refinement. If "setup" is not called prior, "solve" will skip to the triangular solve step. We note that in this solve SuperLU_DIST operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The SUNLinSol_SuperLUDIST module defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_SuperLUDIST`

- `SUNLinSolInitialize_SuperLUDIST` – this sets the `first_factorize` flag to 1 and resets the internal SuperLU_DIST statistics variables.

- `SUNLinSolSetup_SuperLUDIST` – this sets the appropriate SuperLU_DIST options so that a subsequent solve will perform a symbolic and numerical factorization before proceeding with the triangular solves

- `SUNLinSolSolve_SuperLUDIST` – this calls the SuperLU_DIST solve routine to perform factorization (if the setup routine was called prior) and then use the LU factors to solve the linear system.

- `SUNLinSolLastFlag_SuperLUDIST`

- SUNLinSolSpace_SuperLUDIST – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SuperLU_DIST documentation.

- SUNLinSolFree_SuperLUDIST

8.16 The SUNLinSol_SuperLUMT Module

The SUNLinSol_SuperLUMT implementation of the `SUNLinearSolver` class interfaces with the SuperLU_MT library. This is designed to be used with the corresponding SUNMATRIX_SPARSE matrix type, and one of the serial or shared-memory `N_Vector` implementations (NVECTOR_SERIAL, NVECTOR_OPENMP, or NVECTOR_PTHREADS). While these are compatible, it is not recommended to use a threaded vector module with SUNLinSol_SuperLUMT unless it is the NVECTOR_OPENMP module and the SuperLU_MT library has also been compiled with OpenMP.

8.16.1 SUNLinSol_SuperLUMT Usage

The header file to be included when using this module is `sunlinsol/sunlinsol.SuperLUMT.h`. The installed module library to link to is `libsundials_sunlinsolsuperlumt` *.lib* where *.lib* is typically `.so` for shared libraries and `.a` for static libraries.

The module SUNLinSol_SuperLUMT provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_SuperLUMT**(*N_Vector* y, *SUNMatrix* A, int num_threads, *SUNContext* sunctx)

This constructor function creates and allocates memory for a SUNLinSol_SuperLUMT object.

Arguments:

- *y* – a template vector.

- *A* – a template matrix

- *num_threads* – desired number of threads (OpenMP or Pthreads, depending on how SuperLU_MT was installed) to use during the factorization steps.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

If successful, a `SUNLinearSolver` object; otherwise this routine will return NULL.

Notes:

This routine analyzes the input matrix and vector to determine the linear system size and to assess compatibility with the SuperLU_MT library.

This routine will perform consistency checks to ensure that it is called with consistent `N_Vector` and `SUNMatrix` implementations. These are currently limited to the SUNMATRIX_SPARSE matrix type (using either CSR or CSC storage formats) and the NVECTOR_SERIAL, NVECTOR_OPENMP, and NVECTOR_PTHREADS vector types. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

The `num_threads` argument is not checked and is passed directly to SuperLU_MT routines.

int **SUNLinSol_SuperLUMTSetOrdering**(*SUNLinearSolver* S, int ordering_choice)

This function sets the ordering used by SuperLU_MT for reducing fill in the linear solve.

Arguments:

- *S* – the SUNLinSol_SuperLUMT object to update.

- *ordering_choice*:

  0. natural ordering

  1. minimal degree ordering on $A^T A$

  2. minimal degree ordering on $A^T + A$

  3. COLAMD ordering for unsymmetric matrices

  The default is 3 for COLAMD.

  Return value:

  - SUNLS_SUCCESS – option successfully set

  - SUNLS_MEM_NULL – S is NULL

  - SUNLS_ILL_INPUT – invalid `ordering_choice`

For backwards compatibility, we also provide the following wrapper functions, each with identical input and output arguments to the routines that they wrap:

SUNLinearSolver **SUNSuperLUMT**(*N_Vector* y, *SUNMatrix* A, int num_threads)

  Wrapper for *SUNLinSol_SuperLUMT()*.

and

int **SUNSuperLUMTSetOrdering**(*SUNLinearSolver* S, int ordering_choice)

  Wrapper for *SUNLinSol_SuperLUMTSetOrdering()*.

8.16.2 SUNLinSol_SuperLUMT Description

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

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

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

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

- `first_factorize` - flag indicating whether the factorization has ever been performed,

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

- `Gstat` - `GStat_t` object used in solve,

- `perm_r, perm_c` - permutation arrays used in solve,

- `N` - size of the linear system,

- `num_threads` - number of OpenMP/Pthreads threads to use,

- `diag_pivot_thresh` - threshold on diagonal pivoting,

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

- `options` - pointer to SuperLU_MT options structure.

The SUNLinSol_SuperLUMT module is a `SUNLinearSolver` wrapper for the SuperLU_MT sparse matrix factorization and solver library written by X. Sherry Li and collaborators [8, 25, 44]. The package performs matrix factorization using threads to enhance efficiency in shared memory parallel environments. It should be noted that threads are only used in the factorization step. In order to use the SUNLinSol_SuperLUMT interface to SuperLU_MT, it is assumed that SuperLU_MT has been installed on the system prior to installation of SUNDIALS, and that SUNDIALS has been configured appropriately to link with SuperLU_MT (see §11.1.4 for details). Additionally, this wrapper only supports single- and double-precision calculations, and therefore cannot be compiled if SUNDIALS is configured to have *realtype* set to `extended` (see §5.2 for details). Moreover, since the SuperLU_MT library may be installed to support either 32-bit or 64-bit integers, it is assumed that the SuperLU_MT library is installed using the same integer precision as the SUNDIALS *sunindextype* option.

The SuperLU_MT library has a symbolic factorization routine that computes the permutation of the linear system matrix to reduce fill-in on subsequent LU factorizations (using COLAMD, minimal degree ordering on $A^T * A$, minimal degree ordering on $A^T + A$, or natural ordering). Of these ordering choices, the default value in the SUNLinSol_-SuperLUMT module is the COLAMD ordering.

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

- The first time that the "setup" routine is called, it performs the symbolic factorization, followed by an initial numerical factorization.

- On subsequent calls to the "setup" routine, it skips the symbolic factorization, and only refactors the input matrix.

- The "solve" call performs pivoting and forward and backward substitution using the stored SuperLU_MT data structures. We note that in this solve SuperLU_MT operates on the native data arrays for the right-hand side and solution vectors, without requiring costly data copies.

The SUNLinSol_SuperLUMT module defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_SuperLUMT`

- `SUNLinSolInitialize_SuperLUMT` – this sets the `first_factorize` flag to 1 and resets the internal SuperLU_MT statistics variables.

- `SUNLinSolSetup_SuperLUMT` – this performs either a LU factorization or refactorization of the input matrix.

- `SUNLinSolSolve_SuperLUMT` – this calls the appropriate SuperLU_MT solve routine to utilize the LU factors to solve the linear system.

- `SUNLinSolLastFlag_SuperLUMT`

- `SUNLinSolSpace_SuperLUMT` – this only returns information for the storage within the solver *interface*, i.e. storage for the integers `last_flag` and `first_factorize`. For additional space requirements, see the SuperLU_MT documentation.

- `SUNLinSolFree_SuperLUMT`

8.17 The SUNLinSol_cuSolverSp_batchQR Module

The SUNLinSol_cuSolverSp_batchQR implementation of the `SUNLinearSolver` class is designed to be used with the SUNMATRIX_CUSPARSE matrix, and the NVECTOR_CUDA vector. The header file to include when using this module is `sunlinsol/sunlinsol_cusolversp_batchqr.h`. The installed library to link to is `libsundials_-sunlinsolcusolversp.lib` where `.lib` is typically `.so` for shared libraries and `.a` for static libraries.

Warning: The SUNLinearSolver_cuSolverSp_batchQR module is experimental and subject to change.

8.17.1 SUNLinSol_cuSolverSp_batchQR description

The SUNLinearSolver_cuSolverSp_batchQR implementation provides an interface to the batched sparse QR factorization method provided by the NVIDIA cuSOLVER library [5]. The module is designed for solving block diagonal linear systems of the form

$$
\begin{bmatrix}
\mathbf{A_1} & 0 & \cdots & 0 \\
0 & \mathbf{A_2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \mathbf{A_n}
\end{bmatrix}
x_j = b_j
$$

where all block matrices $\mathbf{A_j}$ share the same sparsity pattern. The matrix must be the `SUNMatrix.cuSparse`.

8.17.2 SUNLinSol_cuSolverSp_batchQR functions

The `SUNLinearSolver_cuSolverSp_batchQR` module defines implementations of all "direct" linear solver operations listed in §8.1:

- `SUNLinSolGetType_cuSolverSp_batchQR`

- `SUNLinSolInitialize_cuSolverSp_batchQR` – this sets the `first_factorize` flag to 1

- `SUNLinSolSetup_cuSolverSp_batchQR` – this always copies the relevant SUNMATRIX_SPARSE data to the GPU; if this is the first setup it will perform symbolic analysis on the system

- `SUNLinSolSolve_cuSolverSp_batchQR` – this calls the `cusolverSpXcsrqrsvBatched` routine to perform factorization

- `SUNLinSolLastFlag_cuSolverSp_batchQR`

- `SUNLinSolFree_cuSolverSp_batchQR`

In addition, the module provides the following user-callable routines:

SUNLinearSolver **SUNLinSol_cuSolverSp_batchQR**(*N_Vector* y, *SUNMatrix* A, cusolverHandle_t cusol, *SUNContext* sunctx)

> The function SUNLinSol_cuSolverSp_batchQR creates and allocates memory for a SUNLinearSolver object.

> **Arguments:**

>> - *y* – a vector for checking compatibility with the solver.

>> - *A* – a SUNMATRIX_cuSparse matrix for checking compatibility with the solver.

>> - *cusol* – cuSolverSp object to use.

>> - *sunctx* – the *SUNContext* object (see §4.1)

Return value:

If successful, a SUNLinearSolver object. If either *A* or *y* are incompatible then this routine will return NULL.

Notes:

This routine will perform consistency checks to ensure that it is called with consistent N_Vector and SUN-Matrix implementations. These are currently limited to the SUNMATRIX_CUSPARSE matrix type and the NVECTOR_CUDA vector type. Since the SUNMATRIX_CUSPARSE matrix type is only compatible with the NVECTOR_CUDA the restriction is also in place for the linear solver. As additional compatible matrix and vector implementations are added to SUNDIALS, these will be included within this compatibility check.

void **SUNLinSol_cuSolverSp_batchQR_GetDescription**(*SUNLinearSolver* LS, char **desc)

The function SUNLinSol_cuSolverSp_batchQR_GetDescription accesses the string description of the object (empty by default).

void **SUNLinSol_cuSolverSp_batchQR_SetDescription**(*SUNLinearSolver* LS, const char *desc)

The function SUNLinSol_cuSolverSp_batchQR_SetDescription sets the string description of the object (empty by default).

void **SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace**(*SUNLinearSolver* S, size_t *cuSolverInternal, size_t *cuSolverWorkspace)

The function SUNLinSol_cuSolverSp_batchQR_GetDeviceSpace returns the cuSOLVER batch QR method internal buffer size, in bytes, in the argument cuSolverInternal and the cuSOLVER batch QR workspace buffer size, in bytes, in the agrument cuSolverWorkspace. The size of the internal buffer is proportional to the number of matrix blocks while the size of the workspace is almost independent of the number of blocks.

8.17.3 SUNLinSol_cuSolverSp_batchQR content

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

```
struct _SUNLinearSolverContent_cuSolverSp_batchQR {
  int                last_flag;       /* last return flag                     */
  booleantype        first_factorize; /* is this the first factorization?     */
  size_t             internal_size;   /* size of cusolver buffer for Q and R  */
  size_t             workspace_size;  /* size of cusolver memory for factorization */
  cusolverSpHandle_t cusolver_handle; /* cuSolverSp context                   */
  csrqrInfo_t        info;            /* opaque cusolver data structure       */
  void*              workspace;       /* memory block used by cusolver        */
  const char*        desc;            /* description of this linear solver    */
};
```

8.18 The SUNLINEARSOLVER_GINKGO Module

New in version 6.4.0.

The SUNLINEARSOLVER_GINKGO implementation of the SUNLinearSolver API provides an interface to the linear solvers from the Ginkgo linear algebra library [10]. Since Ginkgo is a modern C++ library, SUNLINEARSOLVER_GINKGO is also written in modern C++ (specifically, C++14). Unlike most other SUNDIALS modules, it is a header only library. To use the SUNLINEARSOLVER_GINKGO SUNLinearSolver, users will need to include sunlinsol/sunlinsol_ginkgo.hpp. The module is meant to be used with the SUNMATRIX_GINKGO module

described in §7.10. Instructions on building SUNDIALS with Ginkgo enabled are given in §11.1.4. For instructions on building and using Ginkgo itself, refer to the Ginkgo website and documentation.

Note: It is assumed that users of this module are aware of how to use Ginkgo. This module does not try to encapsulate Ginkgo linear solvers, rather it provides a lightweight iteroperability layer between Ginkgo and SUNDIALS. Most, if not all, of the Ginkgo linear solver should work with this interface.

8.18.1 Using SUNLINEARSOLVER_GINKGO

After choosing a compatible `N_Vector` (see §7.10.1) and creating a Ginkgo-enabled `SUNMatrix` (see §7.10) to use the SUNLINEARSOLVER_GINKGO module, we first create a Ginkgo stopping criteria object. Importantly, the `sundials::ginkgo::DefaultStop` class provided by SUNDIALS implements a stopping critierion that matches the default SUNDIALS stopping critierion. Namely, it checks if the max iterations (5 by default) were reached or if the absolute residual norm was below a speicified tolerance. The critierion can be created just like any other Ginkgo stopping criteria:

```
auto crit{sundials::ginkgo::DefaultStop::build().with_max_iters(max_iters).on(gko_exec)};
```

Warning: It is *highly* recommended to employ this criterion when using Ginkgo solvers with SUNDIALS, but it is optional. However, to use the Ginkgo multigrid or cbgmres linear solvers, different Ginkgo criterion must be used.

Once we have created our stopping critierion, we create a Ginkgo solver factory object and wrap it in a `sundials::ginkgo::LinearSolver` object. In this example, we create a Ginkgo conjugate gradient solver:

```
using GkoMatrixType = gko::matrix::Csr<sunrealtype, sunindextype>;
using GkoSolverType = gko::solver::Cg<sunrealtype>;

auto gko_solver_factory = gko::share(
   GkoSolverType::build().with_criteria(std::move(crit)).on(gko_exec));

sundials::ginkgo::LinearSolver<GkoSolverType, GkoMatrixType> LS{
   gko_solver_factory, sunctx};
```

Finally, we can pass the instance of `sundials::ginkgo::LinearSolver` to any function expecting a `SUNLinearSolver` object through the implicit conversion operator or explicit conversion function.

```
// Attach linear solver and matrix to CVODE.
//
// Implicit conversion from sundials::ginkgo::LinearSolver<GkoSolverType, GkoMatrixType>
// to a SUNLinearSolver object is done.
//
// For details about creating A see the SUNMATRIX_GINKGO module.
CVodeSetLinearSolver(cvode_mem, LS, A);

// Alternatively with explicit conversion of LS to a SUNLinearSolver
// and A to a SUNMatrix:
CVodeSetLinearSolver(cvode_mem, LS->Convert(), A->Convert());
```

Warning: *SUNLinSolFree()* should never be called on a SUNLinearSolver that was created via conversion from a `sundials::ginkgo::LinearSolver`. Doing so may result in a double free.

8.18.2 SUNLINEARSOLVER_GINKGO API

In this section we list the public API of the `sundials::ginkgo::LinearSolver` class.

template<class **GkoSolverType**, class **GkoMatrixType**>
class **LinearSolver** : public ConvertibleTo<SUNLinearSolver>

> **LinearSolver**() = default;
>> Default constructor - means the solver must be moved to.

> **LinearSolver**(std::shared_ptr<typename *GkoSolverType*::Factory> gko_solver_factory, SUNContext sunctx)
>> Constructs a new LinearSolver from a Ginkgo solver factory.
>>
>> **Parameters**
>>> • **gko_solver_factory** – The Ginkgo solver factory (typically *gko::matrix::<type>::Factory*`)
>>>
>>> • **sunctx** – The SUNDIALS simulation context (*SUNContext*)

> **LinearSolver**(*LinearSolver* &&that_solver) noexcept
>> Move constructor.

> *LinearSolver* &**operator=**(*LinearSolver* &&rhs)
>> Move assignment.

> **~LinearSolver**() override = default
>> Default destructor.

> operator **SUNLinearSolver**() override
>> Implicit conversion to a *SUNLinearSolver*.

> operator **SUNLinearSolver**() const override
>> Implicit conversion to a *SUNLinearSolver*.

> SUNLinearSolver **Convert**() override
>> Explicit conversion to a *SUNLinearSolver*.

> SUNLinearSolver **Convert**() const override
>> Explicit conversion to a *SUNLinearSolver*.

> std::shared_ptr<const gko::Executor> **GkoExec**() const
>> Get the gko::Executor associated with the Ginkgo solver.

> std::shared_ptr<typename *GkoSolverType*::Factory> **GkoFactory**()
>> Get the underlying Ginkgo solver factory.

> *GkoSolverType* ***GkoSolver**()
>> Get the underlying Ginkgo solver.
>>
>> **Note:** This will be *nullptr* until the linear solver setup phase.

int **NumIters**() const

>   Get the number of linear solver iterations in the most recent solve.

sunrealtype **ResNorm**() const

>   Get the residual norm of the solution at the end of the last solve.

>   The type of residual norm depends on the Ginkgo stopping criteria used with the solver. With the De-faultStop criteria this would be the absolute residual 2-norm.

GkoSolverType ***Setup**(*Matrix*<*GkoMatrixType*> *A)

>   Setup the linear system.

>   >   **Parameters**
>   >   >   **A** – the linear system matrix

>   >   **Returns**
>   >   >   Pointer to the Ginkgo solver generated from the factory

gko::LinOp ***Solve**(N_Vector b, N_Vector x, sunrealtype tol)

>   Solve the linear system Ax = b to the specified tolerance.

>   >   **Parameters**
>   >   >   - **b** – the right-hand side vector
>   >   >   - **x** – the solution vector
>   >   >   - **tol** – the tolerance to solve the system to

>   >   **Returns**
>   >   >   gko::LinOp* the solution

8.19 The SUNLINEARSOLVER_KOKKOSDENSE Module

New in version 6.4.0.

The SUNLINEARSOLVER_KOKKOSDENSE *SUNLinearSolver* implementation provides an interface to KokkosKernels [54] linear solvers for dense and batched dense (block-diagonal) systems. Since Kokkos is a modern C++ library, the module is also written in modern C++ (it requires C++14) as a header only library. To utilize this SUNLinearSolver user will need to include sunlinsol/sunlinsol_kokkosdense.hpp. More instructions on building SUNDIALS with Kokkos and KokkosKernels enabled are given in §11.1.4. For instructions on building and using Kokkos and KokkosKernels, refer to the Kokkos and KokkosKernels. documentation.

8.19.1 Using SUNLINEARSOLVER_KOKKOSDENSE

The SUNLINEARSOLVER_KOKKOSDENSE module is defined by the DenseLinearSolver templated class in the sundials::kokkos namespace:

```
template<class ExecSpace = Kokkos::DefaultExecutionSpace,
         class MemSpace = typename ExecSpace::memory_space>
class DenseLinearSolver : public sundials::impl::BaseLinearSolver,
                          public sundials::ConvertibleTo<SUNLinearSolver>
```

To use the SUNLINEARSOLVER_KOKKOSDENSE module, we begin by constructing an instance of a dense linear solver e.g.,

```
// Create a dense linear solver
sundials::kokkos::DenseLinearSolver<> LS{sunctx};
```

Instances of the `DenseLinearSolver` class are implicitly or explicitly (using the *Convert()* method) convertible to a *SUNLinearSolver* e.g.,

```
sundials::kokkos::DenseLinearSolver<> LS{sunctx};
SUNLinearSolver LSA = LS;           // implicit conversion to SUNLinearSolver
SUNLinearSolver LSB = LS.Convert(); // explicit conversion to SUNLinearSolver
```

> **Warning:** *SUNLinSolFree()* should never be called on a `SUNLinearSolver` that was created via conversion from a `sundials::kokkos::DenseLinearSolver`. Doing so may result in a double free.

The SUNLINEARSOLVER_KOKKOSDENSE module is compatible with the NVECTOR_KOKKOS vector module (see §6.14) and SUNMATRIX_KOKKOSDENSE matrix module (see §7.11).

8.19.2 SUNLINEARSOLVER_KOKKOSDENSE API

In this section we list the public API of the `sundials::kokkos::DenseLinearSolver` class.

template<class **ExecSpace** = Kokkos::DefaultExecutionSpace, class **MemSpace** = typename *ExecSpace*::memory_space>
class **DenseLinearSolver** : public sundials::impl::BaseLinearSolver, public sundials::ConvertibleTo<SUNLinearSolver>

> **DenseLinearSolver**() = default;
>
> > Default constructor - means the solver must be moved to.
>
> **DenseLinearSolver**(SUNContext sunctx)
>
> > Constructs a new DenseLinearSolver.
> >
> > > **Parameters**
> > > > **sunctx** – The SUNDIALS simulation context (*SUNContext*)
>
> **DenseLinearSolver**(*DenseLinearSolver* &&that_solver) noexcept
>
> > Move constructor.
>
> *DenseLinearSolver* &**operator=**(*DenseLinearSolver* &&rhs)
>
> > Move assignment.
>
> **~DenseLinearSolver**() override = default
>
> > Default destructor.
>
> **operator SUNLinearSolver**() override
>
> > Implicit conversion to a *SUNLinearSolver*.
>
> **operator SUNLinearSolver**() const override
>
> > Implicit conversion to a *SUNLinearSolver*.
>
> SUNLinearSolver **Convert**() override
>
> > Explicit conversion to a *SUNLinearSolver*.
>
> SUNLinearSolver **Convert**() const override
>
> > Explicit conversion to a *SUNLinearSolver*.

8.20 SUNLinearSolver Examples

There are `SUNLinearSolver` examples that may be installed for each implementation; these make use of the functions in `test_sunlinsol.c`. These example functions show simple usage of the `SUNLinearSolver` family of modules. The inputs to the examples depend on the linear solver type, and are output to `stdout` if the example is run without the appropriate number of command-line arguments.

The following is a list of the example functions in `test_sunlinsol.c`:

- `Test_SUNLinSolGetType`: Verifies the returned solver type against the value that should be returned.

- `Test_SUNLinSolGetID`: Verifies the returned solver identifier against the value that should be returned.

- `Test_SUNLinSolInitialize`: Verifies that `SUNLinSolInitialize` can be called and returns successfully.

- `Test_SUNLinSolSetup`: Verifies that `SUNLinSolSetup` can be called and returns successfully.

- `Test_SUNLinSolSolve`: Given a `SUNMatrix` object A, `N_Vector` objects x and b (where $Ax = b$) and a desired solution tolerance `tol`, this routine clones x into a new vector y, calls `SUNLinSolSolve` to fill y as the solution to $Ay = b$ (to the input tolerance), verifies that each entry in x and y match to within `10*tol`, and overwrites x with y prior to returning (in case the calling routine would like to investigate further).

- `Test_SUNLinSolSetATimes` (iterative solvers only): Verifies that `SUNLinSolSetATimes` can be called and returns successfully.

- `Test_SUNLinSolSetPreconditioner` (iterative solvers only): Verifies that `SUNLinSolSetPreconditioner` can be called and returns successfully.

- `Test_SUNLinSolSetScalingVectors` (iterative solvers only): Verifies that `SUNLinSolSetScalingVectors` can be called and returns successfully.

- `Test_SUNLinSolSetZeroGuess` (iterative solvers only): Verifies that `SUNLinSolSetZeroGuess` can be called and returns successfully.

- `Test_SUNLinSolLastFlag`: Verifies that `SUNLinSolLastFlag` can be called, and outputs the result to `stdout`.

- `Test_SUNLinSolNumIters` (iterative solvers only): Verifies that `SUNLinSolNumIters` can be called, and outputs the result to `stdout`.

- `Test_SUNLinSolResNorm` (iterative solvers only): Verifies that `SUNLinSolResNorm` can be called, and that the result is non-negative.

- `Test_SUNLinSolResid` (iterative solvers only): Verifies that `SUNLinSolResid` can be called.

- `Test_SUNLinSolSpace` verifies that `SUNLinSolSpace` can be called, and outputs the results to `stdout`.

We'll note that these tests should be performed in a particular order. For either direct or iterative linear solvers, `Test_SUNLinSolInitialize` must be called before `Test_SUNLinSolSetup`, which must be called before `Test_SUNLinSolSolve`. Additionally, for iterative linear solvers `Test_SUNLinSolSetATimes`, `Test_SUNLinSolSetPreconditioner` and `Test_SUNLinSolSetScalingVectors` should be called before `Test_SUNLinSolInitialize`; similarly `Test_SUNLinSolNumIters`, `Test_SUNLinSolResNorm` and `Test_SUNLinSolResid` should be called after `Test_SUNLinSolSolve`. These are called in the appropriate order in all of the example problems.

Chapter 9

Nonlinear Algebraic Solvers

SUNDIALS time integration packages are written in terms of generic nonlinear solver operations defined by the SUN-NonlinSol API and implemented by a particular SUNNonlinSol module of type `SUNNonlinearSolver`. Users can supply their own SUNNonlinSol module, or use one of the modules provided with SUNDIALS. Depending on the package, nonlinear solver modules can either target systems presented in a rootfinding ($F(y) = 0$) or fixed-point ($G(y) = y$) formulation. For more information on the formulation of the nonlinear system(s) in CVODE, see §9.2.

The time integrators in SUNDIALS specify a default nonlinear solver module and as such this chapter is intended for users that wish to use a non-default nonlinear solver module or would like to provide their own nonlinear solver implementation. Users interested in using a non-default solver module may skip the description of the SUNNonlinSol API in section §9.1 and proceeded to the subsequent sections in this chapter that describe the SUNNonlinSol modules provided with SUNDIALS.

For users interested in providing their own SUNNonlinSol module, the following section presents the SUNNonlinSol API and its implementation beginning with the definition of SUNNonlinSol functions in the sections §9.1.1, §9.1.2 and §9.1.3. This is followed by the definition of functions supplied to a nonlinear solver implementation in the section §9.1.4. The nonlinear solver return codes are given in the section §9.1.5. The `SUNNonlinearSolver` type and the generic SUNNonlinSol module are defined in the section §9.1.6. Finally, the section §9.1.7 lists the requirements for supplying a custom SUNNonlinSol module. Users wishing to supply their own SUNNonlinSol module are encouraged to use the SUNNonlinSol implementations provided with SUNDIALS as templates for supplying custom nonlinear solver modules.

9.1 The SUNNonlinearSolver API

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

9.1.1 SUNNonlinearSolver core functions

The core nonlinear solver functions consist of two required functions to get the nonlinear solver type (SUNNonlinsSolGetType()) and solve the nonlinear system (*SUNNonlinSolSolve()*). The remaining three functions for nonlinear solver initialization (SUNNonlinSolInitialization()), setup (*SUNNonlinSolSetup()*), and destruction (*SUNNonlinSolFree()*) are optional.

SUNNonlinearSolver_Type **SUNNonlinSolGetType**(*SUNNonlinearSolver* NLS)

This *required* function returns the nonlinear solver type.

Arguments:

- *NLS* – a SUNNonlinSol object.

Return value:

The SUNNonlinSol type identifier (of type int) will be one of the following:

- SUNNONLINEARSOLVER_ROOTFIND – 0, the SUNNonlinSol module solves $F(y) = 0$.

- SUNNONLINEARSOLVER_FIXEDPOINT – 1, the SUNNonlinSol module solves $G(y) = y$.

int **SUNNonlinSolInitialize**(*SUNNonlinearSolver* NLS)

This *optional* function handles nonlinear solver initialization and may perform any necessary memory allocations.

Arguments:

- *NLS* – a SUNNonlinSol object.

Return value:

The return value is zero for a successful call and a negative value for a failure.

Notes:

It is assumed all solver-specific options have been set prior to calling *SUNNonlinSolInitialize()*. SUNNonlinSol implementations that do not require initialization may set this operation to NULL.

int **SUNNonlinSolSetup**(*SUNNonlinearSolver* NLS, *N_Vector* y, void *mem)

This *optional* function performs any solver setup needed for a nonlinear solve.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *y* – the initial guess passed to the nonlinear solver.

- *mem* – the SUNDIALS integrator memory structure.

Return value:

The return value is zero for a successful call and a negative value for a failure.

Notes:

SUNDIALS integrators call SUNonlinSolSetup() before each step attempt. SUNNonlinSol implementations that do not require setup may set this operation to NULL.

int **SUNNonlinSolSolve**(*SUNNonlinearSolver* NLS, *N_Vector* y0, *N_Vector* ycor, *N_Vector* w, *realtype* tol, *booleantype* callLSetup, void *mem)

This *required* function solves the nonlinear system $F(y) = 0$ or $G(y) = y$.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *y0* – the predicted value for the new solution state. This *must* remain unchanged throughout the solution process.

- *ycor* – on input the initial guess for the correction to the predicted state (zero) and on output the final correction to the predicted state.

- *w* – the solution error weight vector used for computing weighted error norms.

- *tol* – the requested solution tolerance in the weighted root-mean-squared norm.

- *callLSetup* – a flag indicating that the integrator recommends for the linear solver setup function to be called.

- *mem* – the SUNDIALS integrator memory structure.

Return value:

The return value is zero for a successul solve, a positive value for a recoverable error (i.e., the solve failed and the integrator should reduce the step size and reattempt the step), and a negative value for an unrecoverable error (i.e., the solve failed the and the integrator should halt and return an error to the user).

int **SUNNonlinSolFree**(*SUNNonlinearSolver* NLS)

This *optional* function frees any memory allocated by the nonlinear solver.

Arguments:

- *NLS* – a SUNNonlinSol object.

Return value:

The return value should be zero for a successful call, and a negative value for a failure. SUNNonlinSol implementations that do not allocate data may set this operation to NULL.

9.1.2 SUNNonlinearSolver "set" functions

The following functions are used to supply nonlinear solver modules with functions defined by the SUNDIALS integrators and to modify solver parameters. Only the routine for setting the nonlinear system defining function (*SUNNonlinSolSetSysFn()*) is required. All other set functions are optional.

int **SUNNonlinSolSetSysFn**(*SUNNonlinearSolver* NLS, *SUNNonlinSolSysFn* SysFn)

This *required* function is used to provide the nonlinear solver with the function defining the nonlinear system. This is the function $F(y)$ in $F(y) = 0$ for SUNNONLINEARSOLVER_ROOTFIND modules or $G(y)$ in $G(y) = y$ for SUNNONLINEARSOLVER_FIXEDPOINT modules.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *SysFn* – the function defining the nonlinear system. See §9.1.4 for the definition of *SUNNonlinSolSysFn*.

Return value:

The return value should be zero for a successful call, and a negative value for a failure.

int **SUNNonlinSolSetLSetupFn**(*SUNNonlinearSolver* NLS, *SUNNonlinSolLSetupFn* SetupFn)

This *optional* function is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver setup function.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *SetupFn* – a wrapper function to the SUNDIALS integrator's linear solver setup function. See §9.1.4 for the definition of *SUNNonlinSolLSetupFn*.

Return value:

The return value should be zero for a successful call, and a negative value for a failure.

Notes:

The *SUNNonlinSolLSetupFn* function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLinSol direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLinSol iterative linear solvers). SUNNonlinSol implementations that do not require solving this system, do not utilize SUNLinSol linear solvers, or use SUNLinSol linear solvers that do not require setup may set this operation to NULL.

int **SUNNonlinSolSetLSolveFn**(*SUNNonlinearSolver* NLS, *SUNNonlinSolLSolveFn* SolveFn)

This *optional* function is called by SUNDIALS integrators to provide the nonlinear solver with access to its linear solver solve function.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *SolveFn* – a wrapper function to the SUNDIALS integrator's linear solver solve function. See §9.1.4 for the definition of *SUNNonlinSolLSolveFn*.

Return value:

The return value should be zero for a successful call, and a negative value for a failure.

Notes:

The *SUNNonlinSolLSolveFn* function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNonlinSol implementations that do not require solving this system or do not use SUNLinSol linear solvers may set this operation to NULL.

int **SUNNonlinSolSetConvTestFn**(*SUNNonlinearSolver* NLS, *SUNNonlinSolConvTestFn* CTestFn, void *ctest_data)

This *optional* function is used to provide the nonlinear solver with a function for determining if the nonlinear solver iteration has converged. This is typically called by SUNDIALS integrators to define their nonlinear convergence criteria, but may be replaced by the user.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *CTestFn* – a SUNDIALS integrator's nonlinear solver convergence test function. See §9.1.4 for the definition of *SUNNonlinSolConvTestFn*.

- *ctest_data* – is a data pointer passed to *CTestFn* every time it is called.

Return value:

The return value should be zero for a successful call, and a negative value for a failure.

Notes:

SUNNonlinSol implementations utilizing their own convergence test criteria may set this function to NULL.

int **SUNNonlinSolSetMaxIters**(*SUNNonlinearSolver* NLS, int maxiters)

This *optional* function sets the maximum number of nonlinear solver iterations. This is typically called by SUNDIALS integrators to define their default iteration limit, but may be adjusted by the user.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *maxiters* – the maximum number of nonlinear iterations.

Return value:

The return value should be zero for a successful call, and a negative value for a failure (e.g., $maxiters < 1$).

9.1.3 SUNNonlinearSolver "get" functions

The following functions allow SUNDIALS integrators to retrieve nonlinear solver statistics. The routines to get the number of iterations in the most recent solve (*SUNNonlinSolGetNumIters()*) and number of convergence failures are optional. The routine to get the current nonlinear solver iteration (*SUNNonlinSolGetCurIter()*) is required when using the convergence test provided by the SUNDIALS integrator or when using an iterative SUNLinSol linear solver module; otherwise *SUNNonlinSolGetCurIter()* is optional.

int **SUNNonlinSolGetNumIters**(*SUNNonlinearSolver* NLS, long int *niters)

> This *optional* function returns the number of nonlinear solver iterations in the most recent solve. This is typically called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.
>
> **Arguments:**
>
> - *NLS* – a SUNNonlinSol object.
>
> - *niters* – the total number of nonlinear solver iterations.
>
> **Return value:**
> > The return value should be zero for a successful call, and a negative value for a failure.

int **SUNNonlinSolGetCurIter**(*SUNNonlinearSolver* NLS, int *iter)

> This function returns the iteration index of the current nonlinear solve. This function is *required* when using SUNDIALS integrator-provided convergence tests or when using an iterative SUNLinSol linear solver module; otherwise it is *optional*.
>
> **Arguments:**
>
> - *NLS* – a SUNNonlinSol object.
>
> - *iter* – the nonlinear solver iteration in the current solve starting from zero.
>
> **Return value:**
> > The return value should be zero for a successful call, and a negative value for a failure.

int **SUNNonlinSolGetNumConvFails**(*SUNNonlinearSolver* NLS, long int *nconvfails)

> This *optional* function returns the number of nonlinear solver convergence failures in the most recent solve. This is typically called by the SUNDIALS integrator to store the nonlinear solver statistics, but may also be called by the user.
>
> **Arguments:**
>
> - *NLS* – a SUNNonlinSol object.
>
> - *nconvfails* – the total number of nonlinear solver convergence failures.
>
> **Return value:**
> > The return value should be zero for a successful call, and a negative value for a failure.

9.1.4 Functions provided by SUNDIALS integrators

To interface with SUNNonlinSol modules, the SUNDIALS integrators supply a variety of routines for evaluating the nonlinear system, calling the SUNLinSol setup and solve functions, and testing the nonlinear iteration for convergence. These integrator-provided routines translate between the user-supplied ODE or DAE systems and the generic interfaces to the nonlinear or linear systems of equations that result in their solution. The functions provided to a SUNNonlinSol module have types defined in the header file sundials/sundials_nonlinearsolver.h; these are also described below.

typedef int (***SUNNonlinSolSysFn**)(*N_Vector* ycor, *N_Vector* F, void *mem)

> These functions evaluate the nonlinear system $F(y)$ for SUNNONLINEARSOLVER_ROOTFIND type modules or $G(y)$ for SUNNONLINEARSOLVER_FIXEDPOINT type modules. Memory for F must by be allocated prior to calling this function. The vector *ycor* will be left unchanged.

> **Arguments:**
>
> > - *ycor* – is the current correction to the predicted state at which the nonlinear system should be evaluated.
> >
> > - *F* – is the output vector containing $F(y)$ or $G(y)$, depending on the solver type.
> >
> > - *mem* – is the SUNDIALS integrator memory structure.

> **Return value:**
>
> > The return value is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

> **Notes:**
>
> > SUNDIALS integrators formulate nonlinear systems as a function of the correction to the predicted solution. On each call to the nonlinear system function the integrator will compute and store the current solution based on the input correction. Additionally, the residual will store the value of the ODE right-hand side function or DAE residual used in computing the nonlinear system. These stored values are then directly used in the integrator-supplied linear solver setup and solve functions as applicable.

typedef int (***SUNNonlinSolLSetupFn**)(*booleantype* jbad, *booleantype* *jcur, void *mem)

> These functions are wrappers to the SUNDIALS integrator's function for setting up linear solves with SUNLinSol modules.

> **Arguments:**
>
> > - *jbad* – is an input indicating whether the nonlinear solver believes that A has gone stale (SUNTRUE) or not (SUNFALSE).
> >
> > - *jcur* – is an output indicating whether the routine has updated the Jacobian A (SUNTRUE) or not (SUNFALSE).
> >
> > - *mem* – is the SUNDIALS integrator memory structure.

> **Return value:**
>
> > The return value is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

> **Notes:**
>
> > The *SUNNonlinSolLSetupFn* function sets up the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$ (when using SUNLinSol direct linear solvers) or calls the user-defined preconditioner setup function (when using SUNLinSol iterative linear solvers). SUNNonlinSol implementations that do not require solving this system, do not utilize SUNLinSol linear solvers, or use SUNLinSol linear solvers that do not require setup may ignore these functions.
> >
> > As discussed in the description of *SUNNonlinSolSysFn*, the linear solver setup function assumes that the nonlinear system function has been called prior to the linear solver setup function as the setup will utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

typedef int (***SUNNonlinSolLSolveFn**)(*N_Vector* b, void *mem)

> These functions are wrappers to the SUNDIALS integrator's function for solving linear systems with SUNLinSol modules.

> **Arguments:**
>
> > - *b* – contains the right-hand side vector for the linear solve on input and the solution to the linear system on output.

- *mem* – is the SUNDIALS integrator memory structure.

Return value:

The return value is zero for a successul solve, a positive value for a recoverable error, and a negative value for an unrecoverable error.

Notes:

The *SUNNonlinSolLSolveFn* function solves the linear system $Ax = b$ where $A = \frac{\partial F}{\partial y}$ is the linearization of the nonlinear residual function $F(y) = 0$. SUNNonlinSol implementations that do not require solving this system or do not use SUNLinSol linear solvers may ignore these functions.

As discussed in the description of *SUNNonlinSolSysFn*, the linear solver solve function assumes that the nonlinear system function has been called prior to the linear solver solve function as the setup may utilize saved values from the nonlinear system evaluation (e.g., the updated solution).

typedef int (***SUNNonlinSolConvTestFn**)(*SUNNonlinearSolver* NLS, *N_Vector* ycor, *N_Vector* del, *realtype* tol, *N_Vector* ewt, void *ctest_data)

These functions are SUNDIALS integrator-specific convergence tests for nonlinear solvers and are typically supplied by each SUNDIALS integrator, but users may supply custom problem-specific versions as desired.

Arguments:

- *NLS* – is the SUNNonlinSol object.

- *ycor* – is the current correction (nonlinear iterate).

- *del* – is the difference between the current and prior nonlinear iterates.

- *tol* – is the nonlinear solver tolerance.

- *ewt* – is the weight vector used in computing weighted norms.

- *ctest_data* – is the data pointer provided to *SUNNonlinSolSetConvTestFn()*.

Return value:

The return value of this routine will be a negative value if an unrecoverable error occurred or one of the following:

- SUN_NLS_SUCCESS – the iteration is converged.

- SUN_NLS_CONTINUE – the iteration has not converged, keep iterating.

- SUN_NLS_CONV_RECVR – the iteration appears to be diverging, try to recover.

Notes:

The tolerance passed to this routine by SUNDIALS integrators is the tolerance in a weighted root-mean-squared norm with error weight vector ewt. SUNNonlinSol modules utilizing their own convergence criteria may ignore these functions.

9.1.5 SUNNonlinearSolver return codes

The functions provided to SUNNonlinSol modules by each SUNDIALS integrator, and functions within the SUNDIALS-provided SUNNonlinSol implementations, utilize a common set of return codes shown in Table 9.1. Here, negative values correspond to non-recoverable failures, positive values to recoverable failures, and zero to a successful call.

Table 9.1: Description of the `SUNNonlinearSolver` return codes.

Name	Value	Description
SUN_NLS_SUCCESS	0	successful call or converged solve
SUN_NLS_CONTINUE	901	the nonlinear solver is not converged, keep iterating
SUN_NLS_CONV_RECVR	902	the nonlinear solver appears to be diverging, try to recover
SUN_NLS_MEM_NULL	-901	a memory argument is NULL
SUN_NLS_MEM_FAIL	-902	a memory access or allocation failed
SUN_NLS_ILL_INPUT	-903	an illegal input option was provided
SUN_NLS_VECTOROP_ERR	-904	a NVECTOR operation failed
SUN_NLS_EXT_FAIL	-905	an external library call returned an error

9.1.6 The generic SUNNonlinearSolver module

SUNDIALS integrators interact with specific SUNNonlinSol implementations through the generic SUNNonlinSol module on which all other SUNNonlinSol implementations are built. The `SUNNonlinearSolver` type is a pointer to a structure containing an implementation-dependent *content* field and an *ops* field. The type `SUNNonlinearSolver` is defined as follows:

typedef struct _generic_SUNNonlinearSolver ***SUNNonlinearSolver**

and the generic structure is defined as

```
struct _generic_SUNNonlinearSolver {
  void *content;
  struct _generic_SUNNonlinearSolver_Ops *ops;
};
```

where the `_generic_SUNNonlinearSolver_Ops` structure is a list of pointers to the various actual nonlinear solver operations provided by a specific implementation. The `_generic_SUNNonlinearSolver_Ops` structure is defined as

```
struct _generic_SUNNonlinearSolver_Ops {
  SUNNonlinearSolver_Type (*gettype)(SUNNonlinearSolver);
  int                     (*initialize)(SUNNonlinearSolver);
  int                     (*setup)(SUNNonlinearSolver, N_Vector, void*);
  int                     (*solve)(SUNNonlinearSolver, N_Vector, N_Vector,
                                   N_Vector, realtype, booleantype, void*);
  int                     (*free)(SUNNonlinearSolver);
  int                     (*setsysfn)(SUNNonlinearSolver, SUNNonlinSolSysFn);
  int                     (*setlsetupfn)(SUNNonlinearSolver, SUNNonlinSolLSetupFn);
  int                     (*setlsolvefn)(SUNNonlinearSolver, SUNNonlinSolLSolveFn);
  int                     (*setctestfn)(SUNNonlinearSolver, SUNNonlinSolConvTestFn,
                                        void*);
  int                     (*setmaxiters)(SUNNonlinearSolver, int);
  int                     (*getnumiters)(SUNNonlinearSolver, long int*);
  int                     (*getcuriter)(SUNNonlinearSolver, int*);
  int                     (*getnumconvfails)(SUNNonlinearSolver, long int*);
};
```

The generic SUNNonlinSol module defines and implements the nonlinear solver operations defined in §9.1.1–§9.1.3. These routines are in fact only wrappers to the nonlinear solver operations provided by a particular SUNNonlinSol implementation, which are accessed through the ops field of the `SUNNonlinearSolver` structure. To illustrate this point we show below the implementation of a typical nonlinear solver operation from the generic SUNNonlinSol module,

namely *SUNNonlinSolSolve()*, which solves the nonlinear system and returns a flag denoting a successful or failed solve:

```c
int SUNNonlinSolSolve(SUNNonlinearSolver NLS,
                      N_Vector y0, N_Vector y,
                      N_Vector w, realtype tol,
                      booleantype callLSetup, void* mem)
{
  return((int) NLS->ops->solve(NLS, y0, y, w, tol, callLSetup, mem));
}
```

9.1.7 Implementing a Custom SUNNonlinearSolver Module

A SUNNonlinSol implementation *must* do the following:

- Specify the content of the SUNNonlinSol module.

- Define and implement the required nonlinear solver operations defined in §9.1.1–§9.1.3. Note that the names of the module routines should be unique to that implementation in order to permit using more than one SUNNonlinSol module (each with different `SUNNonlinearSolver` internal data representations) in the same code.

- Define and implement a user-callable constructor to create a `SUNNonlinearSolver` object.

To aid in the creation of custom `SUNNonlinearSolver` modules, the generic `SUNNonlinearSolver` module provides the utility functions *SUNNonlinSolNewEmpty()* and `SUNNonlinsolFreeEmpty()`. When used in custom `SUNNonlinearSolver` constructors these functions will ease the introduction of any new optional nonlinear solver operations to the `SUNNonlinearSolver` API by ensuring that only required operations need to be set.

SUNNonlinearSolver **SUNNonlinSolNewEmpty**()

> This function allocates a new generic `SUNNonlinearSolver` object and initializes its content pointer and the function pointers in the operations structure to NULL.
>
> **Return value:**
>
> > If successful, this function returns a `SUNNonlinearSolver` object. If an error occurs when allocating the object, then this routine will return NULL.

void **SUNNonlinSolFreeEmpty**(*SUNNonlinearSolver* NLS)

> This routine frees the generic `SUNNonlinearSolver` object, under the assumption that any implementation-specific data that was allocated within the underlying content structure has already been freed. It will additionally test whether the ops pointer is NULL, and, if it is not, it will free it as well.
>
> **Arguments:**
>
> > - *NLS* – a SUNNonlinearSolver object

Additionally, a `SUNNonlinearSolver` implementation *may* do the following:

- Define and implement additional user-callable "set" routines acting on the `SUNNonlinearSolver` object, e.g., for setting various configuration options to tune the performance of the nonlinear solve algorithm.

- Provide additional user-callable "get" routines acting on the `SUNNonlinearSolver` object, e.g., for returning various solve statistics.

9.2 CVODE SUNNonlinearSolver interface

As discussed in §2 each integration step requires the (approximate) solution of a nonlinear system. This system can be formulated as the rootfinding problem

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

or as the fixed-point problem

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

where $a_n \equiv \sum_{i>0} (\alpha_{n,i} y^{n-i} + h_n \beta_{n,i} \dot{y}^{n-i})$.

Rather than solving the above nonlinear systems for the new state y^n CVODE reformulates the above problems to solve for the correction y_{cor} to the predicted new state y_{pred} so that $y^n = y_{pred} + y_{cor}$. The nonlinear systems rewritten in terms of y_{cor} are

$$F(y_{cor}) \equiv y_{cor} - \gamma f(t_n, y^n) - \tilde{a}_n = 0 \tag{9.1}$$

for the rootfinding problem and

$$G(y_{cor}) \equiv \gamma f(t_n, y^n) + \tilde{a}_n = y_{cor} \tag{9.2}$$

for the fixed-point problem.

The nonlinear system functions provided by CVODE to the nonlinear solver module internally update the current value of the new state based on the input correction vector i.e., $y^n = y_{pred} + y_{cor}$. The updated vector y^n is used when calling the ODE right-hand side function and when setting up linear solves (e.g., updating the Jacobian or preconditioner).

CVODE provides several advanced functions that will not be needed by most users, but might be useful for users who choose to provide their own implementation of the *SUNNonlinearSolver* API. For example, such a user might need access to the current value of γ to compute Jacobian data.

int **CVodeGetCurrentGamma**(void *cvode_mem, *realtype* *gamma)

> The function CVodeGetCurrentGamma returns the current value of the scalar $gamma$.
>
> **Arguments:**
>
> - *cvode_mem* – pointer to the CVODE memory block.
>
> - *gamma* – the current value of the scalar γ appearing in the Newton equation $M = I - \gamma J$.
>
> **Return value:**
>
> - CV_SUCCESS – The optional output value has been successfully set.
>
> - CV_MEM_NULL – The CVODE memory block was NULL

int **CVodeGetCurrentState**(void *cvode_mem, *N_Vector* *y)

> The function CVodeGetCurrentState returns the current state vector. When called within the computation of a step (i.e., during a nonlinear solve) this is $y^n = y_{pred} + y_{cor}$. Otherwise this is the current internal solution vector $y(t)$. In either case the corresponding solution time can be obtained from CVodeGetCurrentTime.
>
> **Arguments:**
>
> - *cvode_mem* – pointer to the CVODE memory block.
>
> - *y* – pointer that is set to the current state vector.
>
> **Return value:**
>
> - CV_SUCCESS – The optional output value has been successfully set.
>
> - CV_MEM_NULL – The CVODE memory block was NULL.

int **CVodeGetNonlinearSystemData**(void *cvode_mem, *realtype* *tcur, *N_Vector* *ypred, *N_Vector* *yn, *N_Vector* *fn, *realtype* *gamma, *realtype* *rl1, *N_Vector* *zn1, void **user_data)

The function CVodeGetNonlinearSystemData returns all internal data required to construct the current nonlinear system (9.1) or (9.2).

Arguments:

- *cvode_mem* – pointer to the CVODE memory block.

- *tn* – current value of the independent variable t_n.

- *ypred* – predicted state vector y_{pred} at t_n.

- *yn* – state vector y^n. This vector may be not current and may need to be filled (see the note below).

- *fn* – the right-hand side function evaluated at the current time and state, $f(t_n, y^n)$. This vector may be not current and may need to be filled (see the note below).

- *gamma* – current value of γ.

- *rl1* – a scaling factor used to compute $\tilde{a}_n = $ rl1 * zn1.

- *zn1* – a vector used to compute $\tilde{a}_n = $ rl1 * zn1.

- *user_data* – pointer to the user-defined data structures.

Return value:

- CV_SUCCESS – The optional output values have been successfully set.

- CV_MEM_NULL – The CVODE memory block was NULL.

Notes:

This routine is intended for users who wish to attach a custom *SUNNonlinSolSysFn* to an existing SUNNonlinearSolver object (through a call to *SUNNonlinSolSetSysFn()*) or who need access to nonlinear system data to compute the nonlinear system function as part of a custom SUNNonlinearSolver object. When supplying a custom *SUNNonlinSolSysFn* to an existing SUNNonlinearSolver object, the user should call *CVodeGetNonlinearSystemData()* inside the nonlinear system function to access the requisite data for evaluting the nonlinear system function of their choosing. Additionlly, if the SUNNonlinearSolver object (existing or custom) leverages the *SUNNonlinSolLSetupFn* and/or *SUNNonlinSolLSolveFn* functions supplied by CVODE (through calls to *SUNNonlinSolSetLSetupFn()* and *SUNNonlinSolSetLSolveFn()*, respectively) the vectors yn and fn must be filled in by the user's *SUNNonlinSolSysFn* with the current state and corresponding evaluation of the right-hand side function respectively i.e., $yn = y_{pred} + y_{cor}$ and $f_n = f(t_n, y^n)$ where y_{cor} was the first argument supplied to the *SUNNonlinSolSysFn*. If this function is called as part of a custom linear solver (i.e., the default *SUNNonlinSolSysFn* is used) then the vectors yn and fn are only current when *CVodeGetNonlinearSystemData()* is called after an evaluation of the nonlinear system function.

int **CVodeComputeState**(void *cvode_mem, *N_Vector* ycor, *N_Vector* *yn)

The function computes the current $y(t)$ vector based on stored prediction and the given correction vector from the nonlinear solver i.e., $y^n = y_{pred} + y_{cor}$.

Arguments:

- *cvode_mem* – pointer to the CVODE memory block.

- *ycor* – the correction.

- *yn* – the output vector.

Return value:

- CV_SUCCESS – The optional output value has been successfully set.

 • `CV_MEM_NULL` – The CVODE memory block was `NULL`

9.3 The SUNNonlinSol_Newton implementation

This section describes the SUNNonlinSol implementation of Newton's method. To access the SUNNonlinSol_Newton module, include the header file `sunnonlinsol/sunnonlinsol_newton.h`. We note that the SUNNonlinSol_Newton module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsol-newton` module library.

9.3.1 SUNNonlinSol_Newton description

To find the solution to

$$F(y) = 0 \tag{9.3}$$

given an initial guess $y^{(0)}$, Newton's method computes a series of approximate solutions

$$y^{(m+1)} = y^{(m)} + \delta^{(m+1)}$$

where m is the Newton iteration index, and the Newton update $\delta^{(m+1)}$ is the solution of the linear system

$$A(y^{(m)})\delta^{(m+1)} = -F(y^{(m)}), \tag{9.4}$$

in which A is the Jacobian matrix

$$A \equiv \partial F / \partial y. \tag{9.5}$$

Depending on the linear solver used, the SUNNonlinSol_Newton module will employ either a Modified Newton method or an Inexact Newton method [13, 16, 24, 26, 43]. When used with a direct linear solver, the Jacobian matrix A is held constant during the Newton iteration, resulting in a Modified Newton method. With a matrix-free iterative linear solver, the iteration is an Inexact Newton method.

In both cases, calls to the integrator-supplied *SUNNonlinSolLSetupFn* function are made infrequently to amortize the increased cost of matrix operations (updating A and its factorization within direct linear solvers, or updating the preconditioner within iterative linear solvers). Specifically, SUNNonlinSol_Newton will call the *SUNNonlinSolLSetupFn* function in two instances:

(a) when requested by the integrator (the input `callLSetSetup` is SUNTRUE) before attempting the Newton iteration, or

(b) when reattempting the nonlinear solve after a recoverable failure occurs in the Newton iteration with stale Jacobian information (`jcur` is SUNFALSE). In this case, SUNNonlinSol_Newton will set `jbad` to SUNTRUE before calling the *SUNNonlinSolLSetupFn()* function.

Whether the Jacobian matrix A is fully or partially updated depends on logic unique to each integrator-supplied SUNNonlinSolSetupFn routine. We refer to the discussion of nonlinear solver strategies provided in the package-specific Mathematics section of the documentation for details.

The default maximum number of iterations and the stopping criteria for the Newton iteration are supplied by the SUNDIALS integrator when SUNNonlinSol_Newton is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling the *SUNNonlinSolSetMaxIters()* and/or *SUNNonlinSolSetConvTestFn()* functions after attaching the SUNNonlinSol_Newton object to the integrator.

9.3.2 SUNNonlinSol_Newton functions

The SUNNonlinSol_Newton module provides the following constructor for creating the `SUNnonlinearSolver` object.

SUNNonlinearSolver **SUNNonlinSol_Newton**(*N_Vector* y, *SUNContext* sunctx)

> This creates a `SUNnonlinearSolver` object for use with SUNDIALS integrators to solve nonlinear systems of the form $F(y) = 0$ using Newton's method.
>
> **Arguments:**
>
> - *y* – a template for cloning vectors needed within the solver.
>
> - *sunctx* – the *SUNContext* object (see §4.1)
>
> **Return value:**
>> A SUNNonlinSol object if the constructor exits successfully, otherwise it will be `NULL`.

The SUNNonlinSol_Newton module implements all of the functions defined in §9.1.1–§9.1.3 except for *SUNNonlinSolSetup()*. The SUNNonlinSol_Newton functions have the same names as those defined by the generic SUNNonlinSol API with `_Newton` appended to the function name. Unless using the SUNNonlinSol_Newton module as a standalone nonlinear solver the generic functions defined in §9.1.1–§9.1.3 should be called in favor of the SUNNonlinSol_Newton-specific implementations.

The SUNNonlinSol_Newton module also defines the following user-callable function.

int **SUNNonlinSolGetSysFn_Newton**(*SUNNonlinearSolver* NLS, *SUNNonlinSolSysFn* *SysFn)

> This returns the residual function that defines the nonlinear system.
>
> **Arguments:**
>
> - *NLS* – a SUNNonlinSol object.
>
> - *SysFn* – the function defining the nonlinear system.
>
> **Return value:**
>> The return value should be zero for a successful call, and a negative value for a failure.
>
> **Notes:**
>> This function is intended for users that wish to evaluate the nonlinear residual in a custom convergence test function for the SUNNonlinSol_Newton module. We note that SUNNonlinSol_Newton will not leverage the results from any user calls to *SysFn*.

int **SUNNonlinSolSetInfoFile_Newton**(*SUNNonlinearSolver* NLS, FILE *info_file)

> This sets the output file where all informative (non-error) messages should be directed.
>
> **Arguments:**
>
> - *NLS* – a SUNNonlinSol object.
>
> - *info_file* – **pointer to output file (`stdout` by default);**
>> a NULL input will disable output.
>
> **Return value:**
>
> - `SUN_NLS_SUCCESS` if successful.
>
> - `SUN_NLS_MEM_NULL` if the SUNNonlinSol memory was `NULL`.
>
> - `SUN_NLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled.
>
> **Notes:**
>> This function is intended for users that wish to monitor the nonlinear solver progress. By default, the file pointer is set to `stdout`.

> **Warning:** SUNDIALS must be built with the CMake option `SUNDIALS_LOGGING_LEVEL >= 3` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNNonlinSolSetPrintLevel_Newton**(*SUNNonlinearSolver* NLS, int print_level)

This specifies the level of verbosity of the output.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *print_level* – flag indicating level of verbosity; must be one of:

    - 0, no information is printed (default).

    - 1, for each nonlinear iteration the residual norm is printed.

Return value:

- `SUN_NLS_SUCCESS` if successful.

- `SUN_NLS_MEM_NULL` if the SUNNonlinearSolver memory was `NULL`.

- `SUN_NLS_ILL_INPUT` if SUNDIALS was not built with monitoring enabled, or the print level value was invalid.

Notes:

This function is intended for users that wish to monitor the nonlinear solver progress. By default, the print level is 0.

> **Warning:** SUNDIALS must be built with the CMake option `SUNDIALS_BUILD_WITH_MONITORING` to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

9.3.3 SUNNonlinSol_Newton content

The *content* field of the SUNNonlinSol_Newton module is the following structure.

```
struct _SUNNonlinearSolverContent_Newton {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolLSetupFn   LSetup;
  SUNNonlinSolLSolveFn   LSolve;
  SUNNonlinSolConvTestFn CTest;

  N_Vector    delta;
  booleantype jcur;
  int         curiter;
  int         maxiters;
  long int    niters;
  long int    nconvfails;
  void*       ctest_data;
```

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```
  int        print_level;
  FILE*      info_file;
};
```

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

- `Sys` – the function for evaluating the nonlinear system,

- `LSetup` – the package-supplied function for setting up the linear solver,

- `LSolve` – the package-supplied function for performing a linear solve,

- `CTest` – the function for checking convergence of the Newton iteration,

- `delta` – the Newton iteration update vector,

- `jcur` – the Jacobian status (`SUNTRUE` = current, `SUNFALSE` = stale),

- `curiter` – the current number of iterations in the solve attempt,

- `maxiters` – the maximum number of Newton iterations allowed in a solve,

- `niters` – the total number of nonlinear iterations across all solves,

- `nconvfails` – the total number of nonlinear convergence failures across all solves,

- `ctest_data` – the data pointer passed to the convergence test function,

- `print_level` - controls the amount of information to be printed to the info file,

- `info_file` - the file where all informative (non-error) messages will be directed.

9.4 The SUNNonlinSol_FixedPoint implementation

This section describes the SUNNonlinSol implementation of a fixed point (functional) iteration with optional Anderson acceleration. To access the SUNNonlinSol_FixedPoint module, include the header file `sunnonlinsol/sunnonlinsol_fixedpoint.h`. We note that the SUNNonlinSol_FixedPoint module is accessible from SUNDIALS integrators *without* separately linking to the `libsundials_sunnonlinsolfixedpoint` module library.

9.4.1 SUNNonlinSol_FixedPoint description

To find the solution to

$$G(y) = y \tag{9.6}$$

given an initial guess $y^{(0)}$, the fixed point iteration computes a series of approximate solutions

$$y^{(n+1)} = G(y^{(n)}) \tag{9.7}$$

where n is the iteration index. The convergence of this iteration may be accelerated using Anderson's method [9, 30, 47, 57]. With Anderson acceleration using subspace size m, the series of approximate solutions can be formulated as the linear combination

$$y^{(n+1)} = \beta \sum_{i=0}^{m_n} \alpha_i^{(n)} G(y^{(n-m_n+i)}) + (1 - \beta) \sum_{i=0}^{m_n} \alpha_i^{(n)} y_{n-m_n+i} \tag{9.8}$$

where $m_n = \min\{m, n\}$ and the factors

$$\alpha^{(n)} = (\alpha_0^{(n)}, \ldots, \alpha_{m_n}^{(n)})$$

solve the minimization problem $\min_{\alpha} \|F_n \alpha^T\|_2$ under the constraint that $\sum_{i=0}^{m_n} \alpha_i = 1$ where

$$F_n = (f_{n-m_n}, \ldots, f_n)$$

with $f_i = G(y^{(i)}) - y^{(i)}$. Due to this constraint, in the limit of $m = 0$ the accelerated fixed point iteration formula (9.8) simplifies to the standard fixed point iteration (9.7).

Following the recommendations made in [57], the SUNNonlinSol_FixedPoint implementation computes the series of approximate solutions as

$$y^{(n+1)} = G(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta g_{n-m_n+i} - (1-\beta)(f(y^{(n)}) - \sum_{i=0}^{m_n-1} \gamma_i^{(n)} \Delta f_{n-m_n+i}) \tag{9.9}$$

with $\Delta g_i = G(y^{(i+1)}) - G(y^{(i)})$ and where the factors

$$\gamma^{(n)} = (\gamma_0^{(n)}, \ldots, \gamma_{m_n-1}^{(n)})$$

solve the unconstrained minimization problem $\min_{\gamma} \|f_n - \Delta F_n \gamma^T\|_2$ where

$$\Delta F_n = (\Delta f_{n-m_n}, \ldots, \Delta f_{n-1}),$$

with $\Delta f_i = f_{i+1} - f_i$. The least-squares problem is solved by applying a QR factorization to $\Delta F_n = Q_n R_n$ and solving $R_n \gamma = Q_n^T f_n$.

The acceleration subspace size m is required when constructing the SUNNonlinSol_FixedPoint object. The default maximum number of iterations and the stopping criteria for the fixed point iteration are supplied by the SUNDIALS integrator when SUNNonlinSol_FixedPoint is attached to it. Both the maximum number of iterations and the convergence test function may be modified by the user by calling *SUNNonlinSolSetMaxIters()* and *SUNNonlinSolSet-ConvTestFn()* after attaching the SUNNonlinSol_FixedPoint object to the integrator.

9.4.2 SUNNonlinSol_FixedPoint functions

The SUNNonlinSol_FixedPoint module provides the following constructor for creating the SUNNonlinearSolver object.

SUNNonlinearSolver **SUNNonlinSol_FixedPoint**(*N_Vector* y, int m, *SUNContext* sunctx)

This creates a SUNNonlinearSolver object for use with SUNDIALS integrators to solve nonlinear systems of the form $G(y) = y$.

Arguments:

- *y* – a template for cloning vectors needed within the solver.

- *m* – the number of acceleration vectors to use.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:
A SUNNonlinSol object if the constructor exits successfully, otherwise it will be NULL.

Since the accelerated fixed point iteration (9.7) does not require the setup or solution of any linear systems, the SUN-NonlinSol_FixedPoint module implements all of the functions defined in §9.1.1–§9.1.3 except for the *SUNNonlin-SolSetup()*, *SUNNonlinSolSetLSetupFn()*, and *SUNNonlinSolSetLSolveFn()* functions, that are set to NULL. The SUNNonlinSol_FixedPoint functions have the same names as those defined by the generic SUNNonlinSol API with `_FixedPoint` appended to the function name. Unless using the SUNNonlinSol_FixedPoint module as a standalone nonlinear solver the generic functions defined in §9.1.1–§9.1.3 should be called in favor of the SUNNonlinSol_FixedPoint-specific implementations.

The SUNNonlinSol_FixedPoint module also defines the following user-callable functions.

int **SUNNonlinSolGetSysFn_FixedPoint**(*SUNNonlinearSolver* NLS, *SUNNonlinSolSysFn* *SysFn)

> This returns the fixed-point function that defines the nonlinear system.
>
> **Arguments:**
>
> > - *NLS* – a SUNNonlinSol object.
> >
> > - *SysFn* – the function defining the nonlinear system.
>
> **Return value:**
> > The return value is zero for a successful call, and a negative value for a failure.
>
> **Notes:**
> > This function is intended for users that wish to evaluate the fixed-point function in a custom convergence test function for the SUNNonlinSol_FixedPoint module. We note that SUNNonlinSol_FixedPoint will not leverage the results from any user calls to *SysFn*.

int **SUNNonlinSolSetDamping_FixedPoint**(*SUNNonlinearSolver* NLS, *realtype* beta)

> This sets the damping parameter β to use with Anderson acceleration. By default damping is disabled i.e., $\beta = 1.0$.
>
> **Arguments:**
>
> > - *NLS* – a SUNNonlinSol object.
> >
> > - *beta* – the damping parameter $0 < \beta \leq 1$.
>
> **Return value:**
>
> > - SUN_NLS_SUCCESS if successful.
> >
> > - SUN_NLS_MEM_NULL if NLS was NULL.
> >
> > - SUN_NLS_ILL_INPUT if `beta` was negative.
>
> **Notes:**
> > A `beta` value should satisfy $0 < \beta < 1$ if damping is to be used. A value of one or more will disable damping.

int **SUNNonlinSolSetInfoFile_FixedPoint**(*SUNNonlinearSolver* NLS, FILE *info_file)

> This sets the output file where all informative (non-error) messages should be directed.
>
> **Arguments:**
>
> > - *NLS* – a SUNNonlinSol object.
> >
> > - *info_file* – **pointer to output file (`stdout` by default);**
> >   a NULL input will disable output.
>
> **Return value:**
>
> > - SUN_NLS_SUCCESS if successful.
> >
> > - SUN_NLS_MEM_NULL if NLS was NULL.

- SUN_NLS_ILL_INPUT if SUNDIALS was not built with monitoring enabled.

Notes:

This function is intended for users that wish to monitor the nonlinear solver progress. By default, the file pointer is set to stdout.

> **Warning:** SUNDIALS must be built with the CMake option SUNDIALS_LOGGING_LEVEL >= 3 to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

int **SUNNonlinSolSetPrintLevel_FixedPoint**(*SUNNonlinearSolver* NLS, int print_level)

This specifies the level of verbosity of the output.

Arguments:

- *NLS* – a SUNNonlinSol object.
- *print_level* – flag indicating level of verbosity; must be one of:
    - 0, no information is printed (default).
    - 1, for each nonlinear iteration the residual norm is printed.

Return value:

- SUN_NLS_SUCCESS if successful.
- SUN_NLS_MEM_NULL if NLS was NULL.
- SUN_NLS_ILL_INPUT if SUNDIALS was not built with monitoring enabled, or the print level value was invalid.

Notes:

This function is intended for users that wish to monitor the nonlinear solver progress. By default, the print level is 0.

> **Warning:** SUNDIALS must be built with the CMake option SUNDIALS_BUILD_WITH_MONITORING to utilize this function. See §11.1.2 for more information.

Deprecated since version 6.2.0: Use *SUNLogger_SetInfoFilename()* instead.

9.4.3 SUNNonlinSol_FixedPoint content

The *content* field of the SUNNonlinSol_FixedPoint module is the following structure.

```
struct _SUNNonlinearSolverContent_FixedPoint {

  SUNNonlinSolSysFn      Sys;
  SUNNonlinSolConvTestFn CTest;

  int         m;
  int        *imap;
  realtype   *R;
  booleantype  damping
  realtype     beta
```

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```
    realtype    *gamma;
    realtype    *cvals;
    N_Vector    *df;
    N_Vector    *dg;
    N_Vector    *q;
    N_Vector    *Xvecs;
    N_Vector     yprev;
    N_Vector     gy;
    N_Vector     fold;
    N_Vector     gold;
    N_Vector     delta;
    int          curiter;
    int          maxiters;
    long int     niters;
    long int     nconvfails;
    void        *ctest_data;
    int          print_level;
    FILE*        info_file;
};
```

The following entries of the *content* field are always allocated:

- Sys – function for evaluating the nonlinear system,

- CTest – function for checking convergence of the fixed point iteration,

- yprev – N_Vector used to store previous fixed-point iterate,

- gy – N_Vector used to store $G(y)$ in fixed-point algorithm,

- delta – N_Vector used to store difference between successive fixed-point iterates,

- curiter – the current number of iterations in the solve attempt,

- maxiters – the maximum number of fixed-point iterations allowed in a solve,

- niters – the total number of nonlinear iterations across all solves,

- nconvfails – the total number of nonlinear convergence failures across all solves,

- ctest_data – the data pointer passed to the convergence test function,

- m – number of acceleration vectors,

- print_level - controls the amount of information to be printed to the info file, and

- info_file - the file where all informative (non-error) messages will be directed.

If Anderson acceleration is requested (i.e., $m > 0$ in the call to *SUNNonlinSol_FixedPoint()*), then the following items are also allocated within the *content* field:

- imap – index array used in acceleration algorithm (length m),

- damping – a flag indicating if damping is enabled,

- beta – the damping parameter,

- R – small matrix used in acceleration algorithm (length m*m),

- gamma – small vector used in acceleration algorithm (length m),

- cvals – small vector used in acceleration algorithm (length m+1),

- `df` – array of `N_Vectors` used in acceleration algorithm (length `m`),

- `dg` – array of `N_Vectors` used in acceleration algorithm (length `m`),

- `q` – array of `N_Vectors` used in acceleration algorithm (length `m`),

- `Xvecs` – `N_Vector` pointer array used in acceleration algorithm (length `m+1`),

- `fold` – `N_Vector` used in acceleration algorithm, and

- `gold` – `N_Vector` used in acceleration algorithm.

9.5 The SUNNonlinSol_PetscSNES implementation

This section describes the SUNNonlinSol interface to the PETSc SNES nonlinear solver(s). To enable the SUNonlinSol_PetscSNES module, SUNDIALS must be configured to use PETSc. Instructions on how to do this are given in §11.1.4.7. To access the SUNNonlinSol_PetscSNES module, include the header file `sunnonlinsol/sunnonlinsol_petscsnes.h`. The library to link to is `libsundials_sunnonlinsolpetsc.lib` where `.lib` is typically `.so` for shared libaries and `.a` for static libraries. Users of the SUNNonlinSol_PetscSNES module should also see §6.9 which discusses the NVECTOR interface to the PETSc `Vec` API.

9.5.1 SUNNonlinSol_PetscSNES description

The SUNNonlinSol_PetscSNES implementation allows users to utilize a PETSc SNES nonlinear solver to solve the nonlinear systems that arise in the SUNDIALS integrators. Since SNES uses the KSP linear solver interface underneath it, the SUNNonlinSol_PetscSNES implementation does not interface with SUNDIALS linear solvers. Instead, users should set nonlinear solver options, linear solver options, and preconditioner options through the PETSc SNES, KSP, and PC APIs.

Important usage notes for the SUNNonlinSol_PetscSNES implementation:

- The SUNNonlinSol_PetscSNES implementation handles calling `SNESSetFunction` at construction. The actual residual function $F(y)$ is set by the SUNDIALS integrator when the SUNNonlinSol_PetscSNES object is attached to it. Therefore, a user should not call `SNESSetFunction` on a SNES object that is being used with SUNNonlinSol_PetscSNES. For these reasons it is recommended, although not always necessary, that the user calls *SUNNonlinSol_PetscSNES()* with the new SNES object immediately after calling `SNESCreate`.

- The number of nonlinear iterations is tracked by SUNDIALS separately from the count kept by SNES. As such, the function *SUNNonlinSolGetNumIters()* reports the cumulative number of iterations across the lifetime of the *SUNNonlinearSolver* object.

- Some "converged" and "diverged" convergence reasons returned by SNES are treated as recoverable convergence failures by SUNDIALS. Therefore, the count of convergence failures returned by *SUNNonlinSolGetNumConvFails()* will reflect the number of recoverable convergence failures as determined by SUNDIALS, and may differ from the count returned by `SNESGetNonlinearStepFailures`.

- The SUNNonlinSol_PetscSNES module is not currently compatible with the CVODES or IDAS staggered or simultaneous sensitivity strategies.

9.5.2 SUNNonlinearSolver_PetscSNES functions

The SUNNonlinSol_PetscSNES module provides the following constructor for creating a *SUNNonlinearSolver* object.

SUNNonlinearSolver **SUNNonlinSol_PetscSNES**(*N_Vector* y, SNES snes, *SUNContext* sunctx)

This creates a SUNNonlinSol object that wraps a PETSc SNES object for use with SUNDIALS. This will call SNESSetFunction on the provided SNES object.

Arguments:

- *snes* – a PETSc SNES object.

- *y* – a N_Vector object of type NVECTOR_PETSC that is used as a template for the residual vector.

- *sunctx* – the *SUNContext* object (see §4.1)

Return value:

A SUNNonlinSol object if the constructor exits successfully, otherwise it will be NULL.

> **Warning:** This function calls SNESSetFunction and will overwrite whatever function was previously set. Users should not call SNESSetFunction on the SNES object provided to the constructor.

The SUNNonlinSol_PetscSNES module implements all of the functions defined in §9.1.1–§9.1.3 except for *SUNNonlinSolSetup()*, *SUNNonlinSolSetLSetupFn()*, *SUNNonlinSolSetLSolveFn()*, *SUNNonlinSolSetConvTestFn()*, and *SUNNonlinSolSetMaxIters()*.

The SUNNonlinSol_PetscSNES functions have the same names as those defined by the generic SUNNonlinSol API with _PetscSNES appended to the function name. Unless using the SUNNonlinSol_PetscSNES module as a standalone nonlinear solver the generic functions defined in §9.1.1–§9.1.3 should be called in favor of the SUNNonlinSol_PetscSNES specific implementations.

The SUNNonlinSol_PetscSNES module also defines the following user-callable functions.

int **SUNNonlinSolGetSNES_PetscSNES**(*SUNNonlinearSolver* NLS, SNES *snes)

This gets the SNES object that was wrapped.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *snes* – a pointer to a PETSc SNES object that will be set upon return.

Return value:

The return value (of type int) should be zero for a successful call, and a negative value for a failure.

int **SUNNonlinSolGetPetscError_PetscSNES**(*SUNNonlinearSolver* NLS, PestcErrorCode *error)

This gets the last error code returned by the last internal call to a PETSc API function.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *error* – a pointer to a PETSc error integer that will be set upon return.

Return value:

The return value (of type int) should be zero for a successful call, and a negative value for a failure.

int **SUNNonlinSolGetSysFn_PetscSNES**(*SUNNonlinearSolver* NLS, *SUNNonlinSolSysFn* *SysFn)

This returns the residual function that defines the nonlinear system.

Arguments:

- *NLS* – a SUNNonlinSol object.

- *SysFn* – the function defining the nonlinear system.

Return value:
The return value (of type `int`) should be zero for a successful call, and a negative value for a failure.

9.5.3 SUNNonlinearSolver_PetscSNES content

The *content* field of the SUNNonlinSol_PetscSNES module is the following structure.

```
struct _SUNNonlinearSolverContent_PetscSNES {
  int sysfn_last_err;
  PetscErrorCode petsc_last_err;
  long int nconvfails;
  long int nni;
  void *imem;
  SNES snes;
  Vec r;
  N_Vector y, f;
  SUNNonlinSolSysFn Sys;
};
```

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

- `sysfn_last_err` – last error returned by the system defining function,

- `petsc_last_err` – last error returned by PETSc,

- `nconvfails` – number of nonlinear converge failures (recoverable or not),

- `nni` – number of nonlinear iterations,

- `imem` – SUNDIALS integrator memory,

- `snes` – PETSc SNES object,

- `r` – the nonlinear residual,

- `y` – wrapper for PETSc vectors used in the system function,

- `f` – wrapper for PETSc vectors used in the system function,

- `Sys` – nonlinear system definining function.

Chapter 10

Tools for Memory Management

To support applications which leverage memory pools, or utilize a memory abstraction layer, SUNDIALS provides a set of utilities that we collectively refer to as the SUNMemoryHelper API. The goal of this API is to allow users to leverage operations defined by native SUNDIALS data structures while allowing the user to have finer-grained control of the memory management.

10.1 The SUNMemoryHelper API

This API consists of three new SUNDIALS types: *SUNMemoryType*, *SUNMemory*, and *SUNMemoryHelper*:

typedef struct _SUNMemory ***SUNMemory**

>The `SUNMemory` type is a pointer a structure containing a pointer to actual data (`ptr`), the data memory type, and a flag indicating ownership of that data pointer. This structure is defined as

```
struct _SUNMemory
{
  void*        ptr;
  SUNMemoryType type;
  booleantype   own;
  size_t        bytes;
};
```

enum **SUNMemoryType**

>The `SUNMemoryType` type is an enumeration that defines the supported memory types:

```
typedef enum
{
  SUNMEMTYPE_HOST,      /* pageable memory accessible on the host     */
  SUNMEMTYPE_PINNED,    /* page-locked memory accesible on the host   */
  SUNMEMTYPE_DEVICE,    /* memory accessible from the device          */
  SUNMEMTYPE_UVM        /* memory accessible from the host or device  */
} SUNMemoryType;
```

typedef struct _SUNMemoryHelper ***SUNMemoryHelper**

>The `SUNMemoryHelper` type is a pointer to a structure containing a pointer to the implementation-specific member data (`content`) and a virtual method table of member functions (`ops`). This strucutre is defined as

```
struct _SUNMemoryHelper
{
  void*              content;
  SUNMemoryHelper_Ops ops;
  SUNContext          sunctx;
};
```

typedef struct _SUNMemoryHelper_Ops ***SUNMemoryHelper_Ops**

> The SUNMemoryHelper_Ops type is defined as a pointer to the structure containing the function pointers to the member function implementations. This structure is define as

```
struct _SUNMemoryHelper_Ops
{
  /* operations that implementations are required to provide */
  int (*alloc)(SUNMemoryHelper, SUNMemory* memptr size_t mem_size,
               SUNMemoryType mem_type, void* queue);
  int (*dealloc)(SUNMemoryHelper, SUNMemory mem, void* queue);
  int (*copy)(SUNMemoryHelper, SUNMemory dst, SUNMemory src,
               size_t mem_size, void* queue);

  /* operations that provide default implementations */
  int             (*copyasync)(SUNMemoryHelper, SUNMemory dst,
                               SUNMemory src, size_t mem_size,
                               void* queue);
  int             (*getallocstats)(SUNMemoryHelper, SUNMemoryType mem_type, unsigned long* num_allo
                                   unsigned long* num_deallocations, size_t* bytes_allocated,
                                   size_t* bytes_high_watermark);
  SUNMemoryHelper (*clone)(SUNMemoryHelper);
  int             (*destroy)(SUNMemoryHelper);
};
```

10.1.1 Implementation defined operations

The SUNMemory API defines the following operations that an implementation to must define:

SUNMemory **SUNMemoryHelper_Alloc**(*SUNMemoryHelper* helper, *SUNMemory* *memptr, size_t mem_size, *SUNMemoryType* mem_type, void *queue)

> Allocates a SUNMemory object whose ptr field is allocated for mem_size bytes and is of type mem_type. The new object will have ownership of ptr and will be deallocated when *SUNMemoryHelper_Dealloc()* is called.

> **Arguments:**

> - helper – the SUNMemoryHelper object.

> - memptr – pointer to the allocated SUNMemory.

> - mem_size – the size in bytes of the ptr.

> - mem_type – the SUNMemoryType of the ptr.

> - queue – typically a handle for an object representing an alternate execution stream (e.g., a CUDA/HIP stream or SYCL queue), but it can also be any implementation specific data.

> **Returns:**

> - An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Dealloc**(*SUNMemoryHelper* helper, *SUNMemory* mem, void *queue)

> Deallocates the `mem->ptr` field if it is owned by `mem`, and then deallocates the `mem` object.
>
> **Arguments:**
>
> - `helper` – the SUNMemoryHelper object.
>
> - `mem` – the SUNMemory object.
>
> - `queue` – typically a handle for an object representing an alternate execution stream (e.g., a CUDA/HIP stream or SYCL queue), but it can also be any implementation specific data.
>
> **Returns:**
>
> - An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Copy**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t mem_size, void *queue)

> Synchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object should use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.
>
> **Arguments:**
>
> - `helper` – the SUNMemoryHelper object.
>
> - `dst` – the destination memory to copy to.
>
> - `src` – the source memory to copy from.
>
> - `mem_size` – the number of bytes to copy.
>
> - `queue` – typically a handle for an object representing an alternate execution stream (e.g., a CUDA/HIP stream or SYCL queue), but it can also be any implementation specific data.
>
> **Returns:**
>
> - An `int` flag indicating success (zero) or failure (non-zero).

10.1.2 Utility Functions

The SUNMemoryHelper API defines the following functions which do not require a SUNMemoryHelper instance:

SUNMemory **SUNMemoryHelper_Alias**(*SUNMemory* mem1)

> Returns a SUNMemory object whose `ptr` field points to the same address as `mem1`. The new object *will not* have ownership of `ptr`, therefore, it will not free `ptr` when *SUNMemoryHelper_Dealloc()* is called.
>
> **Arguments:**
>
> - `mem1` – a SUNMemory object.
>
> **Returns:**
>
> - A SUNMemory object or NULL if an error occurs.

SUNMemory **SUNMemoryHelper_Wrap**(void *ptr, *SUNMemoryType* mem_type)

> Returns a SUNMemory object whose `ptr` field points to the `ptr` argument passed to the function. The new object *will not* have ownership of `ptr`, therefore, it will not free `ptr` when *SUNMemoryHelper_Dealloc()* is called.
>
> **Arguments:**
>
> - `ptr` – the data pointer to wrap in a SUNMemory object.
>
> - `mem_type` – the SUNMemoryType of the `ptr`.

Returns:

- A SUNMemory object or NULL if an error occurs.

SUNMemoryHelper **SUNMemoryHelper_NewEmpty**()

Returns an empty SUNMemoryHelper. This is useful for building custom SUNMemoryHelper implementations.

Returns:

- A SUNMemoryHelper object or NULL if an error occurs.

int **SUNMemoryHelper_CopyOps**(*SUNMemoryHelper* src, *SUNMemoryHelper* dst)

Copies the ops field of src to the ops field of dst. This is useful for building custom SUNMemoryHelper implementations.

Arguments:

- src – the object to copy from.

- dst – the object to copy to.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_GetAllocStats**(*SUNMemoryHelper* helper, *SUNMemoryType* mem_type, unsigned long *num_allocations, unsigned long *num_deallocations, size_t *bytes_allocated, size_t *bytes_high_watermark)

Returns statistics about the allocations performed with the helper.

Arguments:

- helper – the SUNMemoryHelper object.

- mem_type – the SUNMemoryType to get stats for.

- num_allocations – (output argument) number of allocations done through the helper.

- num_deallocations – (output argument) number of deallocations done through the helper.

- bytes_allocated – (output argument) total number of bytes allocated through the helper at the moment this function is called.

- bytes_high_watermark – (output argument) max number of bytes allocated through the helper at any moment in the lifetime of the helper.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

10.1.3 Implementation overridable operations with defaults

In addition, the SUNMemoryHelper API defines the following *optionally overridable* operations which an implementation may define:

int **SUNMemoryHelper_CopyAsync**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t mem_size, void *queue)

Asynchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object should use the memory types of dst and src to determine the appropriate transfer type necessary. The ctx argument is used when a different execution stream needs to be provided to perform the copy in, e.g. with CUDA this would be a cudaStream_t.

Arguments:

- helper – the SUNMemoryHelper object.

- dst – the destination memory to copy to.

- src – the source memory to copy from.

- mem_size – the number of bytes to copy.

- queue – typically a handle for an object representing an alternate execution stream (e.g., a CUDA/HIP stream or SYCL queue), but it can also be any implementation specific data.

Returns:

An int flag indicating success (zero) or failure (non-zero).

Note: If this operation is not defined by the implementation, then *SUNMemoryHelper_Copy()* will be used.

SUNMemoryHelper **SUNMemoryHelper_Clone**(*SUNMemoryHelper* helper)

Clones the SUNMemoryHelper object itself.

Arguments:

- helper – the SUNMemoryHelper object to clone.

Returns:

- A SUNMemoryHelper object.

Note: If this operation is not defined by the implementation, then the default clone will only copy the SUNMemoryHelper_Ops structure stored in helper->ops, and not the helper->content field.

---

int **SUNMemoryHelper_Destroy**(*SUNMemoryHelper* helper)

Destroys (frees) the SUNMemoryHelper object itself.

Arguments:

- helper – the SUNMemoryHelper object to destroy.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

Note: If this operation is not defined by the implementation, then the default destroy will only free the helper->ops field and the helper itself. The helper->content field will not be freed.

10.1.4 Implementing a custom SUNMemoryHelper

A particular implementation of the SUNMemoryHelper API must:

- Define and implement the required operations. Note that the names of these routines should be unique to that implementation in order to permit using more than one SUNMemoryHelper module in the same code.

- Optionally, specify the *content* field of SUNMemoryHelper.

- Optionally, define and implement additional user-callable routines acting on the newly defined SUNMemoryHelper.

An example of a custom SUNMemoryHelper is given in `examples/utilities/custom_memory_helper.h`.

10.2 The SUNMemoryHelper_Cuda Implementation

The SUNMemoryHelper_Cuda module is an implementation of the `SUNMemoryHelper` API that interfaces to the NVIDIA [4] library. The implementation defines the constructor

SUNMemoryHelper **SUNMemoryHelper_Cuda**(*SUNContext* sunctx)

>   Allocates and returns a `SUNMemoryHelper` object for handling CUDA memory if successful. Otherwise it returns `NULL`.

10.2.1 SUNMemoryHelper_Cuda API Functions

The implementation provides the following operations defined by the `SUNMemoryHelper` API:

SUNMemory **SUNMemoryHelper_Alloc_Cuda**(*SUNMemoryHelper* helper, *SUNMemory* memptr, size_t mem_size, *SUNMemoryType* mem_type, void *queue)

>   Allocates a `SUNMemory` object whose `ptr` field is allocated for `mem_size` bytes and is of type `mem_type`. The new object will have ownership of `ptr` and will be deallocated when *SUNMemoryHelper_Dealloc()* is called.

>   **Arguments:**
>
>   - `helper` – the SUNMemoryHelper object.
>   - `memptr` – pointer to the allocated SUNMemory.
>   - `mem_size` – the size in bytes of the `ptr`.
>   - `mem_type` – the SUNMemoryType of the `ptr`. Supported values are:
>   - `SUNMEMTYPE_HOST` – memory is allocated with a call to `malloc`.
>   - `SUNMEMTYPE_PINNED` – memory is allocated with a call to `cudaMallocHost`.
>   - `SUNMEMTYPE_DEVICE` – memory is allocated with a call to `cudaMalloc`.
>   - `SUNMEMTYPE_UVM` – memory is allocated with a call to `cudaMallocManaged`.
>   - `queue` – currently unused.
>
>   **Returns:**
>
>   - An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Dealloc_Cuda**(*SUNMemoryHelper* helper, *SUNMemory* mem, void *queue)

>   Deallocates the `mem->ptr` field if it is owned by `mem`, and then deallocates the `mem` object.

>   **Arguments:**
>
>   - `helper` – the SUNMemoryHelper object.
>   - `mem` – the SUNMemory object.
>   - `queue` – currently unused.
>
>   **Returns:**
>
>   - An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Copy_Cuda**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t
mem_size, void *queue)

Synchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments:

- `helper` – the SUNMemoryHelper object.
- `dst` – the destination memory to copy to.
- `src` – the source memory to copy from.
- `mem_size` – the number of bytes to copy.
- `queue` – currently unused.

Returns:

- An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_CopyAsync_Cuda**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t
mem_size, void *queue)

Asynchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments:

- `helper` – the SUNMemoryHelper object.
- `dst` – the destination memory to copy to.
- `src` – the source memory to copy from.
- `mem_size` – the number of bytes to copy.
- `queue` – the `cudaStream_t` handle for the stream that the copy will be performed on.

Returns:

- An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_GetAllocStats_Cuda**(*SUNMemoryHelper* helper, *SUNMemoryType* mem_type, unsigned
long *num_allocations, unsigned long *num_deallocations, size_t
*bytes_allocated, size_t *bytes_high_watermark)

Returns statistics about memory allocations performed with the helper.

Arguments:

- `helper` – the SUNMemoryHelper object.
- `mem_type` – the SUNMemoryType to get stats for.
- `num_allocations` – (output argument) number of memory allocations done through the helper.
- `num_deallocations` – (output argument) number of memory deallocations done through the helper.
- `bytes_allocated` – (output argument) total number of bytes allocated through the helper at the moment this function is called.
- `bytes_high_watermark` – (output argument) max number of bytes allocated through the helper at any moment in the lifetime of the helper.

Returns:

• An int flag indicating success (zero) or failure (non-zero).

10.3 The SUNMemoryHelper_Hip Implementation

The SUNMemoryHelper_Hip module is an implementation of the SUNMemoryHelper API that interfaces to the AMD ROCm HIP library [1]. The implementation defines the constructor

SUNMemoryHelper **SUNMemoryHelper_Hip**(*SUNContext* sunctx)

  Allocates and returns a SUNMemoryHelper object for handling HIP memory if successful. Otherwise it returns NULL.

10.3.1 SUNMemoryHelper_Hip API Functions

The implementation provides the following operations defined by the SUNMemoryHelper API:

SUNMemory **SUNMemoryHelper_Alloc_Hip**(*SUNMemoryHelper* helper, *SUNMemory* memptr, size_t mem_size, *SUNMemoryType* mem_type, void *queue)

  Allocates a SUNMemory object whose ptr field is allocated for mem_size bytes and is of type mem_type. The new object will have ownership of ptr and will be deallocated when *SUNMemoryHelper_Dealloc()* is called.

  Arguments:

  • helper – the SUNMemoryHelper object.

  • memptr – pointer to the allocated SUNMemory.

  • mem_size – the size in bytes of the ptr.

  • mem_type – the SUNMemoryType of the ptr. Supported values are:

    – SUNMEMTYPE_HOST – memory is allocated with a call to malloc.

    – SUNMEMTYPE_PINNED – memory is allocated with a call to hipMallocHost.

    – SUNMEMTYPE_DEVICE – memory is allocated with a call to hipMalloc.

    – SUNMEMTYPE_UVM – memory is allocated with a call to hipMallocManaged.

  • queue – currently unused.

  Returns:

  • An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Dealloc_Hip**(*SUNMemoryHelper* helper, *SUNMemory* mem, void *queue)

  Deallocates the mem->ptr field if it is owned by mem, and then deallocates the mem object.

  Arguments:

  • helper – the SUNMemoryHelper object.

  • mem – the SUNMemory object.

  Returns:

  • An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Copy_Hip**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t mem_size, void *queue)

Synchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments:

- `helper` – the SUNMemoryHelper object.

- `dst` – the destination memory to copy to.

- `src` – the source memory to copy from.

- `mem_size` – the number of bytes to copy.

Returns:

- An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_CopyAsync_Hip**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t mem_size, void *queue)

Asynchronously copies `mem_size` bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The `helper` object will use the memory types of `dst` and `src` to determine the appropriate transfer type necessary.

Arguments:

- `helper` – the SUNMemoryHelper object.

- `dst` – the destination memory to copy to.

- `src` – the source memory to copy from.

- `mem_size` – the number of bytes to copy.

- `queue` – the `hipStream_t` handle for the stream that the copy will be performed on.

Returns:

- An `int` flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_GetAllocStats_Hip**(*SUNMemoryHelper* helper, *SUNMemoryType* mem_type, unsigned long *num_allocations, unsigned long *num_deallocations, size_t *bytes_allocated, size_t *bytes_high_watermark)

Returns statistics about memory allocations performed with the helper.

Arguments:

- `helper` – the SUNMemoryHelper object.

- `mem_type` – the SUNMemoryType to get stats for.

- `num_allocations` – (output argument) number of memory allocations done through the helper.

- `num_deallocations` – (output argument) number of memory deallocations done through the helper.

- `bytes_allocated` – (output argument) total number of bytes allocated through the helper at the moment this function is called.

- `bytes_high_watermark` – (output argument) max number of bytes allocated through the helper at any moment in the lifetime of the helper.

Returns:

- An `int` flag indicating success (zero) or failure (non-zero).

10.4 The SUNMemoryHelper_Sycl Implementation

The SUNMemoryHelper_Sycl module is an implementation of the SUNMemoryHelper API that interfaces to the SYCL abstraction layer. The implementation defines the constructor

SUNMemoryHelper **SUNMemoryHelper_Sycl**(*SUNContext* sunctx)

>   Allocates and returns a SUNMemoryHelper object for handling SYCL memory using the provided queue. Otherwise it returns NULL.

10.4.1 SUNMemoryHelper_Sycl API Functions

The implementation provides the following operations defined by the SUNMemoryHelper API:

SUNMemory **SUNMemoryHelper_Alloc_Sycl**(*SUNMemoryHelper* helper, *SUNMemory* memptr, size_t mem_size, *SUNMemoryType* mem_type, void *queue)

>   Allocates a SUNMemory object whose ptr field is allocated for mem_size bytes and is of type mem_type. The new object will have ownership of ptr and will be deallocated when *SUNMemoryHelper_Dealloc()* is called.
>
>   **Arguments:**
>
>   - helper – the SUNMemoryHelper object.
>
>   - memptr – pointer to the allocated SUNMemory.
>
>   - mem_size – the size in bytes of the ptr.
>
>   - mem_type – the SUNMemoryType of the ptr. Supported values are:
>
>   - SUNMEMTYPE_HOST – memory is allocated with a call to malloc.
>
>   - SUNMEMTYPE_PINNED – memory is allocated with a call to sycl::malloc_host.
>
>   - SUNMEMTYPE_DEVICE – memory is allocated with a call to sycl::malloc_device.
>
>   - SUNMEMTYPE_UVM – memory is allocated with a call to sycl::malloc_shared.
>
>   - queue – the sycl::queue handle for the stream that the allocation will be performed on.
>
>   **Returns:**
>
>   - An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Dealloc_Sycl**(*SUNMemoryHelper* helper, *SUNMemory* mem, void *queue)

>   Deallocates the mem->ptr field if it is owned by mem, and then deallocates the mem object.
>
>   **Arguments:**
>
>   - helper – the SUNMemoryHelper object.
>
>   - mem – the SUNMemory object.
>
>   - queue – the sycl::queue handle for the queue that the deallocation will be performed on.
>
>   **Returns:**
>
>   - An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_Copy_Sycl**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t mem_size, void *queue)

>   Synchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object will use the memory types of dst and src to determine the appropriate transfer type necessary.

Arguments:

- helper – the SUNMemoryHelper object.
- dst – the destination memory to copy to.
- src – the source memory to copy from.
- mem_size – the number of bytes to copy.
- queue – the sycl::queue handle for the queue that the copy will be performed on.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_CopyAsync_Sycl**(*SUNMemoryHelper* helper, *SUNMemory* dst, *SUNMemory* src, size_t
mem_size, void *queue)

Asynchronously copies mem_size bytes from the the source memory to the destination memory. The copy can be across memory spaces, e.g. host to device, or within a memory space, e.g. host to host. The helper object will use the memory types of dst and src to determine the appropriate transfer type necessary.

Arguments:

- helper – the SUNMemoryHelper object.
- dst – the destination memory to copy to.
- src – the source memory to copy from.
- mem_size – the number of bytes to copy.
- queue – the sycl::queue handle for the queue that the copy will be performed on.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

int **SUNMemoryHelper_GetAllocStats_Sycl**(*SUNMemoryHelper* helper, *SUNMemoryType* mem_type, unsigned
long *num_allocations, unsigned long *num_deallocations, size_t
*bytes_allocated, size_t *bytes_high_watermark)

Returns statistics about memory allocations performed with the helper.

Arguments:

- helper – the SUNMemoryHelper object.
- mem_type – the SUNMemoryType to get stats for.
- num_allocations – (output argument) number of memory allocations done through the helper.
- num_deallocations – (output argument) number of memory deallocations done through the helper.
- bytes_allocated – (output argument) total number of bytes allocated through the helper at the moment this function is called.
- bytes_high_watermark – (output argument) max number of bytes allocated through the helper at any moment in the lifetime of the helper.

Returns:

- An int flag indicating success (zero) or failure (non-zero).

Chapter 11

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 -zxf SOLVER-X.Y.Z.tar.gz
```

This will extract source files under a directory `SOLVER-X.Y.Z`.

Starting with version 2.6.0 of SUNDIALS, CMake is the only supported method of installation. The explanations of the installation procedure begin with a few common observations:

1. The remainder of this chapter will follow these conventions:

   `SOLVERDIR` is the directory `SOLVER-X.Y.Z` created above; i.e. the directory containing the SUNDIALS sources.

   `BUILDDIR` is the (temporary) directory under which SUNDIALS is built.

   `INSTDIR` is the directory under which the SUNDIALS exported header files and libraries will be installed. Typically, header files are exported under a directory `INSTDIR/include` while libraries are installed under `INSTDIR/lib`, with `INSTDIR` specified at configuration time.

2. For SUNDIALS' CMake-based installation, in-source builds are prohibited; in other words, the build directory `BUILDDIR` can **not** be the same as `SOLVERDIR` and such an attempt will lead to an error. This prevents "polluting" the source tree and allows efficient builds for different configurations and/or options.

3. The installation directory `INSTDIR` can not be the same as the source directory `SOLVERDIR`.

4. 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.)

Further details on the CMake-based installation procedures, instructions for manual compilation, and a roadmap of the resulting installed libraries and exported header files, are provided in §11.1 and §11.2.

11.1 CMake-based installation

CMake-based installation provides a platform-independent build system. CMake can generate Unix and Linux Makefiles, as well as KDevelop, Visual Studio, and (Apple) XCode project files from the same configuration file. In addition, CMake also provides a GUI front end and which allows an interactive build and installation process.

The SUNDIALS build process requires CMake version 3.12.0 or higher and a working C compiler. On Unix-like operating systems, it also requires Make (and `curses`, including its development libraries, for the GUI front end to CMake, `ccmake` or `cmake-gui`), while on Windows it requires Visual Studio. While many Linux distributions offer CMake, the version included may be out of date. CMake adds new features regularly, 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` or `cmake-gui` (depending on the version of CMake), 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.

11.1.1 Configuring, building, and installing on Unix-like systems

The default CMake configuration will build all included solvers and associated examples and will build static and shared libraries. The INSTDIR defaults to `/usr/local` and can be changed by setting the `CMAKE_INSTALL_PREFIX` variable. Support for FORTRAN and all other options are disabled.

CMake can be used from the command line with the `cmake` command, or from a `curses`-based GUI by using the `ccmake` command, or from a wxWidgets or QT based GUI by using the `cmake-gui` command. Examples for using both text and graphical 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 (...)/INSTDIR
$ mkdir (...)/BUILDDIR
$ cd (...)/BUILDDIR
```

11.1.1.1 Building with the GUI

Using CMake with the `ccmake` GUI follows the general process:

1. Select and modify values, run configure (`c` key)

2. New values are denoted with an asterisk

3. 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

4. Repeat until all values are set as desired and the generate option is available (`g` key)

5. Some variables (advanced variables) are not visible right away; to see advanced variables, toggle to advanced mode (`t` key)

6. To search for a variable press the `/` key, and to repeat the search, press the `n` key

Using CMake with the `cmake-gui` GUI follows a similar process:

1. Select and modify values, click `Configure`

2. The first time you click `Configure`, make sure to pick the appropriate generator (the following will assume generation of Unix Makfiles).

3. New values are highlighted in red

4. To set a variable, click on or move the cursor to the variable and press enter

   - If it is a boolean (`ON/OFF`) it will check/uncheck the box

   - If it is string or file, it will allow editing of the string. Additionally, an ellipsis button will appear `...` on the far right of the entry. Clicking this button will bring up the file or directory selection dialog.

   - For files and directories, the `<tab>` key can be used to complete

5. Repeat until all values are set as desired and click the `Generate` button

6. Some variables (advanced variables) are not visible right away; to see advanced variables, click the `advanced` button

To build the default configuration using the curses GUI, from the `BUILDDIR` enter the `ccmake` command and point to the `SOLVERDIR`:

```
$ ccmake (...)/SOLVERDIR
```

Similarly, to build the default configuration using the wxWidgets GUI, from the `BUILDDIR` enter the `cmake-gui` command and point to the `SOLVERDIR`:

```
$ cmake-gui (...)/SOLVERDIR
```

The default curses configuration screen is shown in the following figure.

The default `INSTDIR` for both SUNDIALS and the corresponding examples can be changed by setting the `CMAKE_-INSTALL_PREFIX` and the `EXAMPLES_INSTALL_PATH` as shown in the following figure.

Pressing the `g` key or clicking `generate` 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
```

or for a faster parallel build (e.g. using 4 threads), you can run

```
$ make -j 4
```

To install SUNDIALS in the installation directory specified in the configuration, simply run:

```
$ make install
```

```
                                    Page 1 of 1
BUILD_ARKODE                       *ON
BUILD_CVODE                        *ON
BUILD_CVODES                       *ON
BUILD_EXAMPLES                     *ON
BUILD_IDA                          *ON
BUILD_IDAS                         *ON
BUILD_KINSOL                       *ON
BUILD_SHARED_LIBS                  *ON
BUILD_STATIC_LIBS                  *ON
BUILD_TESTING                      *ON
CMAKE_BUILD_TYPE                   *
CMAKE_CXX_COMPILER                 */usr/bin/c++
CMAKE_CXX_FLAGS                    *
CMAKE_C_COMPILER                   */usr/bin/cc
CMAKE_C_FLAGS                      *
CMAKE_INSTALL_LIBDIR               *lib64
CMAKE_INSTALL_PREFIX               */usr/local
ENABLE_CUDA                        *OFF
ENABLE_FORTRAN                     *OFF
ENABLE_HYPRE                       *OFF
ENABLE_KLU                         *OFF
ENABLE_LAPACK                      *OFF
ENABLE_MPI                         *OFF
ENABLE_OPENMP                      *OFF
ENABLE_OPENMP_DEVICE               *OFF
ENABLE_PETSC                       *OFF
ENABLE_PTHREAD                     *OFF
ENABLE_RAJA                        *OFF
ENABLE_SUPERLUDIST                 *OFF
ENABLE_SUPERLUMT                   *OFF
ENABLE_TRILINOS                    *OFF
EXAMPLES_ENABLE_C                  *ON
EXAMPLES_ENABLE_CXX                *ON
EXAMPLES_INSTALL                   *ON
EXAMPLES_INSTALL_PATH              */usr/local/examples
SUNDIALS_BUILD_WITH_MONITORING     *OFF
SUNDIALS_INDEX_SIZE                *64
SUNDIALS_PRECISION                 *DOUBLE
USE_GENERIC_MATH                   *ON
USE_XSDK_DEFAULTS                  *OFF




BUILD_ARKODE: Build the ARKODE library
Press [enter] to edit option Press [d] to delete an entry             CMake Version 3.12.1
Press [c] to configure
Press [h] for help          Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Fig. 11.1: 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.

```
                                    Page 1 of 1
BUILD_ARKODE                     *ON
BUILD_CVODE                      *ON
BUILD_CVODES                     *ON
BUILD_EXAMPLES                   *ON
BUILD_IDA                        *ON
BUILD_IDAS                       *ON
BUILD_KINSOL                     *ON
BUILD_SHARED_LIBS                *ON
BUILD_STATIC_LIBS                *ON
BUILD_TESTING                    *ON
CMAKE_BUILD_TYPE                 *
CMAKE_CXX_COMPILER               */usr/bin/c++
CMAKE_CXX_FLAGS                  *
CMAKE_C_COMPILER                 */usr/bin/cc
CMAKE_C_FLAGS                    *
CMAKE_INSTALL_LIBDIR             *lib64
CMAKE_INSTALL_PREFIX             */usr/casc/sundials/instdir
ENABLE_CUDA                      *OFF
ENABLE_FORTRAN                   *OFF
ENABLE_HYPRE                     *OFF
ENABLE_KLU                       *OFF
ENABLE_LAPACK                    *OFF
ENABLE_MPI                       *OFF
ENABLE_OPENMP                    *OFF
ENABLE_OPENMP_DEVICE             *OFF
ENABLE_PETSC                     *OFF
ENABLE_PTHREAD                   *OFF
ENABLE_RAJA                      *OFF
ENABLE_SUPERLUDIST               *OFF
ENABLE_SUPERLUMT                 *OFF
ENABLE_TRILINOS                  *OFF
EXAMPLES_ENABLE_C                *ON
EXAMPLES_ENABLE_CXX              *ON
EXAMPLES_INSTALL                 *ON
EXAMPLES_INSTALL_PATH            */usr/casc/sundials/instdir/examples
SUNDIALS_BUILD_WITH_MONITORING   *OFF
SUNDIALS_INDEX_SIZE              *64
SUNDIALS_PRECISION               *DOUBLE
USE_GENERIC_MATH                 *ON
USE_XSDK_DEFAULTS                *OFF



EXAMPLES_INSTALL_PATH: Output directory for installing example files
Press [enter] to edit option Press [d] to delete an entry              CMake Version 3.12.1
Press [c] to configure
Press [h] for help          Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

Fig. 11.2: Changing the INSTDIR for SUNDIALS and corresponding EXAMPLES.

11.1.1.2 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
```

11.1.2 Configuration options (Unix/Linux)

A complete list of all available options for a CMake-based SUNDIALS configuration is provide below. Note that the default values shown are for a typical configuration on a Linux system and are provided as illustration only.

BUILD_ARKODE

> Build the ARKODE library

> Default: `ON`

BUILD_CVODE

> Build the CVODE library

> Default: `ON`

BUILD_CVODES

> Build the CVODES library

> Default: `ON`

BUILD_IDA

> Build the IDA library

> Default: `ON`

BUILD_IDAS

> Build the IDAS library

> Default: `ON`

BUILD_KINSOL

> Build the KINSOL library

> Default: `ON`

BUILD_SHARED_LIBS

> Build shared libraries

> Default: `ON`

BUILD_STATIC_LIBS

> Build static libraries

> Default: `ON`

CMAKE_BUILD_TYPE

Choose the type of build, options are: `None`, `Debug`, `Release`, `RelWithDebInfo`, and `MinSizeRel`

Default:

Note: Specifying a build type will trigger the corresponding build type specific compiler flag options below which will be appended to the flags set by `CMAKE_<language>_FLAGS`.

CMAKE_C_COMPILER

C compiler

Default: `/usr/bin/cc`

CMAKE_C_FLAGS

Flags for C compiler

Default:

CMAKE_C_FLAGS_DEBUG

Flags used by the C compiler during debug builds

Default: `-g`

CMAKE_C_FLAGS_MINSIZEREL

Flags used by the C compiler during release minsize builds

Default: `-Os -DNDEBUG`

CMAKE_C_FLAGS_RELEASE

Flags used by the C compiler during release builds

Default: `-O3 -DNDEBUG`

CMAKE_C_STANDARD

The C standard to build C parts of SUNDIALS with.

Default: 99

Options: 90, 99, 11, 17.

CMAKE_C_EXTENSIONS

Enable compiler specific C extensions.

Default: `OFF`

CMAKE_CXX_COMPILER

C++ compiler

Default: `/usr/bin/c++`

Note: A C++ compiler is only required when a feature requiring C++ is enabled (e.g., CUDA, HIP, SYCL, RAJA, etc.) or the C++ examples are enabled.

All SUNDIALS solvers can be used from C++ applications without setting any additional configuration options.

CMAKE_CXX_FLAGS

Flags for C++ compiler

Default:

CMAKE_CXX_FLAGS_DEBUG

> Flags used by the C++ compiler during debug builds

> Default: `-g`

CMAKE_CXX_FLAGS_MINSIZEREL

> Flags used by the C++ compiler during release minsize builds

> Default: `-Os -DNDEBUG`

CMAKE_CXX_FLAGS_RELEASE

> Flags used by the C++ compiler during release builds

> Default: `-O3 -DNDEBUG`

CMAKE_CXX_STANDARD

> The C++ standard to build C++ parts of SUNDIALS with.

> Default: 11

> Options: 98, 11, 14, 17, 20.

CMAKE_CXX_EXTENSIONS

> Enable compiler specific C++ extensions.

> Default: `OFF`

CMAKE_Fortran_COMPILER

> Fortran compiler

> Default: `/usr/bin/gfortran`

> **Note:** Fortran support (and all related options) are triggered only if either Fortran-C support (`BUILD_FORTRAN_-MODULE_INTERFACE`) or LAPACK (`ENABLE_LAPACK`) support is enabled.

CMAKE_Fortran_FLAGS

> Flags for Fortran compiler

> Default:

CMAKE_Fortran_FLAGS_DEBUG

> Flags used by the Fortran compiler during debug builds

> Default: `-g`

CMAKE_Fortran_FLAGS_MINSIZEREL

> Flags used by the Fortran compiler during release minsize builds

> Default: `-Os`

CMAKE_Fortran_FLAGS_RELEASE

> Flags used by the Fortran compiler during release builds

> Default: `-O3`

CMAKE_INSTALL_LIBDIR

> The directory under which libraries will be installed.

> Default: Set based on the system: `lib`, `lib64`, or `lib/<multiarch-tuple>`

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.

ENABLE_CUDA

Build the SUNDIALS CUDA modules.

Default: `OFF`

CMAKE_CUDA_ARCHITECTURES

Specifies the CUDA architecture to compile for.

Default: `sm_30`

ENABLE_XBRAID

Enable or disable the ARKStep + XBraid interface.

Default: `OFF`

Note: See additional information on building with *XBraid* enabled in §11.1.4.

EXAMPLES_ENABLE_C

Build the SUNDIALS C examples

Default: `ON`

EXAMPLES_ENABLE_CXX

Build the SUNDIALS C++ examples

Default: `OFF`

EXAMPLES_ENABLE_CUDA

Build the SUNDIALS CUDA examples

Default: `OFF`

Note: You need to enable CUDA support to build these examples.

EXAMPLES_ENABLE_F2003

Build the SUNDIALS Fortran2003 examples

Default: `ON` (if `BUILD_FORTRAN_MODULE_INTERFACE` is `ON`)

EXAMPLES_INSTALL

Install example files

Default: `ON`

Note: This option is triggered when any of the SUNDIALS example programs are enabled (`EXAMPLES_-ENABLE_<language>` is `ON`). If the user requires installation of example programs then the sources and sample

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output files for all SUNDIALS modules that are currently enabled will be exported to the directory specified by `EXAMPLES_INSTALL_PATH`. A CMake configuration script will also be automatically generated and exported to the same directory. Additionally, if the configuration is done under a Unix-like system, makefiles for the compilation of the example programs (using the installed SUNDIALS libraries) will be automatically generated and exported to the directory specified by `EXAMPLES_INSTALL_PATH`.

`EXAMPLES_INSTALL_PATH`

Output directory for installing example files

Default: `/usr/local/examples`

Note: The actual default value for this option will be an `examples` subdirectory created under `CMAKE_IN-STALL_PREFIX`.

`BUILD_FORTRAN_MODULE_INTERFACE`

Enable Fortran 2003 interface

Default: `OFF`

`ENABLE_GINKGO`

Enable interfaces to the Ginkgo linear algebra library.

Default: `OFF`

`Ginkgo_DIR`

Path to the Ginkgo installation.

Default: None

`SUNDIALS_GINKGO_BACKENDS`

Semi-colon separated list of Ginkgo target architecutres/executors to build for. Options currenty supported are REF (the Ginkgo reference executor), OMP, CUDA, HIP, and DPC++.

Default: "REF;OMP"

`ENABLE_KOKKOS`

Enable the Kokkos based vector.

Default: `OFF`

`Kokkos_DIR`

Path to the Kokkos installation.

Default: None

`ENABLE_KOKKOS_KERNELS`

Enable the Kokkos based dense matrix and linear solver.

Default: `OFF`

`KokkosKernels_DIR`

Path to the Kokkos-Kernels installation.

Default: None

`ENABLE_HIP`

Enable HIP Support

Default: `OFF`

AMDGPU_TARGETS

Specify which AMDGPU processor(s) to target.

Default: None

ENABLE_HYPRE

Flag to enable *hypre* support

Default: `OFF`

Note: See additional information on building with *hypre* enabled in §11.1.4.

HYPRE_INCLUDE_DIR

Path to *hypre* header files

Default: none

HYPRE_LIBRARY

Path to *hypre* installed library files

Default: none

ENABLE_KLU

Enable KLU support

Default: `OFF`

Note: See additional information on building with KLU enabled in §11.1.4.

KLU_INCLUDE_DIR

Path to SuiteSparse header files

Default: none

KLU_LIBRARY_DIR

Path to SuiteSparse installed library files

Default: none

ENABLE_LAPACK

Enable LAPACK support

Default: `OFF`

Note: Setting this option to `ON` will trigger additional CMake options. See additional information on building with LAPACK enabled in §11.1.4.

LAPACK_LIBRARIES

LAPACK (and BLAS) libraries

Default: `/usr/lib/liblapack.so;/usr/lib/libblas.so`

Note: CMake will search for libraries in your `LD_LIBRARY_PATH` prior to searching default system paths.

ENABLE_MAGMA

Enable MAGMA support.

Default: OFF

> **Note:** Setting this option to ON will trigger additional options related to MAGMA.

MAGMA_DIR

Path to the root of a MAGMA installation.

Default: none

SUNDIALS_MAGMA_BACKENDS

Which MAGMA backend to use under the SUNDIALS MAGMA interface.

Default: CUDA

ENABLE_MPI

Enable MPI support. This will build the parallel nvector and the MPI-aware version of the ManyVector library.

Default: OFF

> **Note:** Setting this option to ON will trigger several additional options related to MPI.

MPI_C_COMPILER

mpicc program

Default:

MPI_CXX_COMPILER

mpicxx program

Default:

> **Note:** This option is triggered only if MPI is enabled (ENABLE_MPI is ON) and C++ examples are enabled (EXAMPLES_ENABLE_CXX is ON). All SUNDIALS solvers can be used from C++ MPI applications by default without setting any additional configuration options other than ENABLE_MPI.

MPI_Fortran_COMPILER

mpif90 program

Default:

> **Note:** This option is triggered only if MPI is enabled (ENABLE_MPI is ON) and Fortran-C support is enabled (EXAMPLES_ENABLE_F2003 is ON).

MPIEXEC_EXECUTABLE

Specify the executable for running MPI programs

Default: mpirun

> **Note:** This option is triggered only if MPI is enabled (ENABLE_MPI is ON).

ENABLE_ONEMKL

    Enable oneMKL support.

    Default: `OFF`

ONEMKL_DIR

    Path to oneMKL installation.

    Default: none

SUNDIALS_ONEMKL_USE_GETRF_LOOP

    This advanced debugging option replaces the batched LU factorization with a loop over each system in the batch and a non-batched LU factorization.

    Default: OFF

SUNDIALS_ONEMKL_USE_GETRS_LOOP

    This advanced debugging option replaces the batched LU solve with a loop over each system in the batch and a non-batched solve.

    Default: OFF

ENABLE_OPENMP

    Enable OpenMP support (build the OpenMP NVector)

    Default: `OFF`

ENABLE_PETSC

    Enable PETSc support

    Default: `OFF`

    Note: See additional information on building with PETSc enabled in §11.1.4.

PETSC_DIR

    Path to PETSc installation

    Default: none

PETSC_LIBRARIES

    Semi-colon separated list of PETSc link libraries. Unless provided by the user, this is autopopulated based on the PETSc installation found in `PETSC_DIR`.

    Default: none

PETSC_INCLUDES

    Semi-colon separated list of PETSc include directroies. Unless provided by the user, this is autopopulated based on the PETSc installation found in `PETSC_DIR`.

    Default: none

ENABLE_PTHREAD

    Enable Pthreads support (build the Pthreads NVector)

    Default: `OFF`

ENABLE_RAJA

    Enable RAJA support.

    Default: OFF

Note: You need to enable CUDA or HIP in order to build the RAJA vector module.

SUNDIALS_RAJA_BACKENDS

If building SUNDIALS with RAJA support, this sets the RAJA backend to target. Values supported are CUDA, HIP, or SYCL.

Default: CUDA

ENABLE_SUPERLUDIST

Enable SuperLU_DIST support

Default: OFF

Note: See additional information on building wtih SuperLU_DIST enabled in §11.1.4.

SUPERLUDIST_DIR

Path to SuperLU_DIST installation.

Default: none

SUPERLUDIST_OpenMP

Enable SUNDIALS support for SuperLU_DIST built with OpenMP

Default: none

Note: SuperLU_DIST must be built with OpenMP support for this option to function. Additionally the environment variable OMP_NUM_THREADS must be set to the desired number of threads.

SUPERLUDIST_INCLUDE_DIRS

List of include paths for SuperLU_DIST (under a typical SuperLU_DIST install, this is typically the SuperLU_-DIST SRC directory)

Default: none

Note: This is an advanced option. Prefer to use *SUPERLUDIST_DIR*.

SUPERLUDIST_LIBRARIES

Semi-colon separated list of libraries needed for SuperLU_DIST

Default: none

Note: This is an advanced option. Prefer to use *SUPERLUDIST_DIR*.

SUPERLUDIST_INCLUDE_DIR

Path to SuperLU_DIST header files (under a typical SuperLU_DIST install, this is typically the SuperLU_DIST SRC directory)

Default: none

Note: This is an advanced option. This option is deprecated. Use *SUPERLUDIST_INCLUDE_DIRS*.

SUPERLUDIST_LIBRARY_DIR

Path to SuperLU_DIST installed library files

Default: none

Note: This option is deprecated. Use *SUPERLUDIST_DIR*.

ENABLE_SUPERLUMT

Enable SuperLU_MT support

Default: `OFF`

Note: See additional information on building with SuperLU_MT enabled in §11.1.4.

SUPERLUMT_INCLUDE_DIR

Path to SuperLU_MT header files (under a typical SuperLU_MT install, this is typically the SuperLU_MT SRC directory)

Default: none

SUPERLUMT_LIBRARY_DIR

Path to SuperLU_MT installed library files

Default: none

SUPERLUMT_THREAD_TYPE

Must be set to Pthread or OpenMP, depending on how SuperLU_MT was compiled.

Default: Pthread

ENABLE_SYCL

Enable SYCL support.

Default: OFF

Note: CMake does not currently support autodetection of SYCL compilers and `CMAKE_CXX_COMPILER` must be set to a valid SYCL compiler. At present the only supported SYCL compilers are the Intel oneAPI compilers i.e., `dpcpp` and `icpx`. When using `icpx` the `-fsycl` flag and any ahead of time compilation flags must be added to `CMAKE_CXX_FLAGS`.

SUNDIALS_SYCL_2020_UNSUPPORTED

This advanced option disables the use of *some* features from the SYCL 2020 standard in SUNDIALS libraries and examples. This can be used to work around some cases of incomplete compiler support for SYCL 2020.

Default: OFF

SUNDIALS_LOGGING_LEVEL

Set the maximum logging level for the SUNLogger runtime API. The higher this is set, the more output that may be logged, and the more performance may degrade. The options are:

- `0` – no logging
- `1` – log errors
- `2` – log errors + warnings
- `3` – log errors + warnings + informational output

- 4 – log errors + warnings + informational output + debug output

- 5 – log all of the above and even more (e.g. vector valued variables may be logged)

Default: 0

SUNDIALS_LOGGING_ENABLE_MPI

Enables MPI support in the SUNLogger runtime API. I.e., makes the logger MPI aware and capable of outputting only on specific ranks.

Default: `OFF`

Note: The logger may be used in an MPI application without MPI support turned on, but it will output on all ranks.

SUNDIALS_BUILD_WITH_MONITORING

Build SUNDIALS with capabilties for fine-grained monitoring of solver progress and statistics. This is primarily useful for debugging.

Default: OFF

Warning: Building with monitoring may result in minor performance degradation even if monitoring is not utilized.

SUNDIALS_BUILD_WITH_PROFILING

Build SUNDIALS with capabilties for fine-grained profiling. This requires POSIX timers or the Windows `profileapi.h` timers.

Default: OFF

Warning: Profiling will impact performance, and should be enabled judiciously.

ENABLE_CALIPER

Enable CALIPER support

Default: OFF

Note: Using Caliper requires setting *SUNDIALS_BUILD_WITH_PROFILING* to `ON`.

CALIPER_DIR

Path to the root of a Caliper installation

Default: None

ENABLE_ADIAK

Enable Adiak support

Default: OFF

adiak_DIR

Path to the root of an Adiak installation

Default: None

SUNDIALS_F77_FUNC_CASE

Specify the case to use in the Fortran name-mangling scheme, options are: `lower` or `upper`

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (`lower`) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_UNDERSCORES` must also be set.

SUNDIALS_F77_FUNC_UNDERSCORES

Specify the number of underscores to append in the Fortran name-mangling scheme, options are: `none`, `one`, or `two`

Default:

Note: The build system will attempt to infer the Fortran name-mangling scheme using the Fortran compiler. This option should only be used if a Fortran compiler is not available or to override the inferred or default (`one`) scheme if one can not be determined. If used, `SUNDIALS_F77_FUNC_CASE` must also be set.

SUNDIALS_INDEX_TYPE

Integer type used for SUNDIALS indices. The size must match the size provided for the `SUNDIALS_INDEX_SIZE` option.

Default: Automatically determined based on *SUNDIALS_INDEX_SIZE*

Note: In past SUNDIALS versions, a user could set this option to `INT64_T` to use 64-bit integers, or `INT32_T` to use 32-bit integers. Starting in SUNDIALS 3.2.0, these special values are deprecated. For SUNDIALS 3.2.0 and up, a user will only need to use the *SUNDIALS_INDEX_SIZE* option in most cases.

SUNDIALS_INDEX_SIZE

Integer size (in bits) used for indices in SUNDIALS, options are: `32` or `64`

Default: `64`

Note: The build system tries to find an integer type of appropriate size. Candidate 64-bit integer types are (in order of preference): `int64_t`, `__int64`, `long long`, and `long`. Candidate 32-bit integers are (in order of preference): `int32_t`, `int`, and `long`. The advanced option, *SUNDIALS_INDEX_TYPE* can be used to provide a type not listed here.

SUNDIALS_MATH_LIBRARY

The standard C math library (e.g., `libm`) to link with.

Default: `-lm` on Unix systems, none otherwise

SUNDIALS_PRECISION

The floating-point precision used in SUNDIALS packages and class implementations, options are: `double`, `single`, or `extended`

Default: `double`

SUNDIALS_INSTALL_CMAKEDIR

      Installation directory for the SUNDIALS cmake files (relative to *CMAKE_INSTALL_PREFIX*).

      Default: CMAKE_INSTALL_PREFIX/cmake/sundials

USE_GENERIC_MATH

      Link to *SUNDIALS_MATH_LIBRARY*, which defaults to libm on Unix systems.

      Default: ON

      Note: This option is deprecated. Use *SUNDIALS_MATH_LIBRARY*.

XBRAID_DIR

      The root directory of the XBraid installation.

      Default: OFF

XBRAID_INCLUDES

      Semi-colon separated list of XBraid include directories. Unless provided by the user, this is autopopulated based on the XBraid installation found in XBRAID_DIR.

      Default: none

XBRAID_LIBRARIES

      Semi-colon separated list of XBraid link libraries. Unless provided by the user, this is autopopulated based on the XBraid installation found in XBRAID_DIR.

      Default: none

USE_XSDK_DEFAULTS

      Enable xSDK (see https://xsdk.info for more information) default configuration settings. This sets CMAKE_-BUILD_TYPE to Debug, SUNDIALS_INDEX_SIZE to 32 and SUNDIALS_PRECISION to double.

      Default: OFF

11.1.3 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 mpif90 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 \
> -DENABLE_MPI=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 \
```

```
> -DENABLE_MPI=ON \
> -DEXAMPLES_INSTALL=OFF \
> /home/myname/sundials/srcdir

% make install
```

11.1.4 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.

11.1.4.1 Building with Ginkgo

Ginkgo is a high-performance linear algebra library for manycore systems, with a focus on solving sparse linear systems. It is implemented using modern C++ (you will need at least a C++14 compliant compiler to build it), with GPU kernels implemented in CUDA (for NVIDIA devices), HIP (for AMD devices) and SYCL/DPC++ (for Intel devices and other supported hardware). To enable Ginkgo in SUNDIALS, set the *ENABLE_GINKGO* to ON and provide the path to the root of the Ginkgo installation in *Ginkgo_DIR*. Additionally, *SUNDIALS_GINKGO_BACKENDS* must be set to a list of Ginkgo target architecutres/executors. E.g.,

```
% cmake \
> -DENABLE_GINKGO=ON \
> -DGinkgo_DIR=/path/to/ginkgo/installation \
> -DSUNDIALS_GINKGO_BACKENDS="REF;OMP;CUDA" \
> /home/myname/sundials/srcdir
```

The SUNDIALS interfaces to Ginkgo are not compatible with *SUNDIALS_PRECISION* set to `extended`.

11.1.4.2 Building with Kokkos

Kokkos is a modern C++ (requires at least C++14) programming model for witting performance portable code for multi-core CPU and GPU-based systems including NVIDIA, AMD, and Intel accelerators. To enable Kokkos in SUNDIALS, set the *ENABLE_KOKKOS* to ON and provide the path to the root of the Kokkos installation in *Kokkos_DIR*. Additionally, the Kokkos-Kernels library provides common computational kernels for linear algebra. To enable Kokkos-Kernels in SUNDIALS, set the *ENABLE_KOKKOS_KERNELS* to ON and provide the path to the root of the Kokkos-Kernels installation in *KokkosKernels_DIR* e.g.,

```
% cmake \
> -DENABLE_KOKKOS=ON \
> -DKokkos_DIR=/path/to/kokkos/installation \
> -DENABLE_KOKKOS_KERNELS=ON \
> -DKokkosKernels_DIR=/path/to/kokkoskernels/installation \
> /home/myname/sundials/srcdir
```

Note: The minimum supported version of Kokkos-Kernels 3.7.00.

11.1.4.3 Building with LAPACK

To enable LAPACK, set the `ENABLE_LAPACK` option to `ON`. If the directory containing the LAPACK library is in the `LD_LIBRARY_PATH` environment variable, CMake will set the `LAPACK_LIBRARIES` variable accordingly, otherwise CMake will attempt to find the LAPACK library in standard system locations. To explicitly tell CMake what library to use, the `LAPACK_LIBRARIES` variable can be set to the desired libraries required for LAPACK.

```
% cmake \
> -DCMAKE_INSTALL_PREFIX=/home/myname/sundials/instdir \
> -DEXAMPLES_INSTALL_PATH=/home/myname/sundials/instdir/examples \
> -DENABLE_LAPACK=ON \
> -DLAPACK_LIBRARIES=/mylapackpath/lib/libblas.so;/mylapackpath/lib/liblapack.so \
> /home/myname/sundials/srcdir

% make install
```

Note: If a working Fortran compiler is not available to infer the Fortran name-mangling scheme, the options `SUNDI-ALS_F77_FUNC_CASE` and `SUNDIALS_F77_FUNC_UNDERSCORES` *must* be set in order to bypass the check for a Fortran compiler and define the name-mangling scheme. The defaults for these options in earlier versions of SUNDIALS were `lower` and `one`, respectively.

SUNDIALS has been tested with OpenBLAS 0.3.18.

11.1.4.4 Building with KLU

KLU is a software package for the direct solution of sparse nonsymmetric linear systems of equations that arise in circuit simulation and is part of SuiteSparse, a suite of sparse matrix software. The library is developed by Texas A&M University and is available from the SuiteSparse GitHub repository.

To enable KLU, set `ENABLE_KLU` 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`, `CO-LAMD_LIBRARY_DIR`, and `KLU_LIBRARY`.

SUNDIALS has been tested with SuiteSparse version 5.10.1.

11.1.4.5 Building with SuperLU_DIST

SuperLU_DIST is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations in a distributed memory setting. The library is developed by Lawrence Berkeley National Laboratory and is available from the SuperLU_DIST GitHub repository.

To enable SuperLU_DIST, set *ENABLE_SUPERLUDIST* to `ON`, set *SUPERLUDIST_DIR* to the path where SuperLU_DIST is installed. If SuperLU_DIST was built with OpenMP then the option *SUPERLUDIST_OpenMP* and *ENABLE_OPENMP* should be set to `ON`.

SUNDIALS supports SuperLU_DIST v7.0.0 – v8.x.x and has been tested with v7.2.0 and v8.1.0.

11.1.4.6 Building with SuperLU_MT

SuperLU_MT is a general purpose library for the direct solution of large, sparse, nonsymmetric systems of linear equations on shared memory parallel machines. The library is developed by Lawrence Berkeley National Laboratory and is available from the SuperLU_MT GitHub repository.

To enable SuperLU_MT, set `ENABLE_SUPERLUMT` to `ON`, set `SUPERLUMT_INCLUDE_DIR` to the SRC path of the SuperLU_MT installation, and set the variable `SUPERLUMT_LIBRARY_DIR` to the `lib` path of the SuperLU_MT installation. At the same time, the variable `SUPERLUMT_LIBRARIES` must be set to a semi-colon separated list of other libraries SuperLU_MT depends on. For example, if SuperLU_MT was build with an external blas library, then include the full path to the blas library in this list. Additionally, the variable `SUPERLUMT_THREAD_TYPE` must be set to either `Pthread` or `OpenMP`.

Do not mix thread types when building SUNDIALS solvers. If threading is enabled for SUNDIALS by having either `ENABLE_OPENMP` or `ENABLE_PTHREAD` set to `ON` then SuperLU_MT should be set to use the same threading type.

SUNDIALS has been tested with SuperLU_MT version 3.1.

11.1.4.7 Building with PETSc

The Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of data structures and routines for simulating applications modeled by partial differential equations. The library is developed by Argonne National Laboratory and is available from the PETSc GitLab repository.

To enable PETSc, set `ENABLE_PETSC` to `ON`, and set `PETSC_DIR` to the path of the PETSc installation. Alternatively, a user can provide a list of include paths in `PETSC_INCLUDES` and a list of complete paths to the PETSc libraries in `PETSC_LIBRARIES`.

SUNDIALS is regularly tested with the latest PETSc versions, specifically up to version 3.18.1 as of SUNDIALS version v6.7.0. SUNDIALS requires PETSc 3.5.0 or newer.

11.1.4.8 Building with *hypre*

hypre is a library of high performance preconditioners and solvers featuring multigrid methods for the solution of large, sparse linear systems of equations on massively parallel computers. The library is developed by Lawrence Livermore National Laboratory and is available from the hypre GitHub repository.

To enable *hypre*, set `ENABLE_HYPRE` to `ON`, set `HYPRE_INCLUDE_DIR` to the `include` path of the *hypre* installation, and set the variable `HYPRE_LIBRARY_DIR` to the `lib` path of the *hypre* installation.

Note: SUNDIALS must be configured so that `SUNDIALS_INDEX_SIZE` is compatible with `HYPRE_BigInt` in the *hypre* installation.

SUNDIALS is regularly tested with the latest versions of *hypre*, specifically up to version 2.26.0 as of SUNDIALS version v6.7.0.

11.1.4.9 Building with MAGMA

The Matrix Algebra on GPU and Multicore Architectures (MAGMA) project provides a dense linear algebra library similar to LAPACK but targeting heterogeneous architectures. The library is developed by the University of Tennessee and is available from the UTK webpage.

To enable the SUNDIALS MAGMA interface set `ENABLE_MAGMA` to `ON`, `MAGMA_DIR` to the MAGMA installation path, and `SUNDIALS_MAGMA_BACKENDS` to the desired MAGMA backend to use with SUNDIALS e.g., `CUDA` or `HIP`.

SUNDIALS has been tested with MAGMA version v2.6.1 and v2.6.2.

11.1.4.10 Building with oneMKL

The Intel oneAPI Math Kernel Library (oneMKL) includes CPU and DPC++ interfaces for LAPACK dense linear algebra routines. The SUNDIALS oneMKL interface targets the DPC++ routines, to utilize the CPU routine see §11.1.4.3.

To enable the SUNDIALS oneMKL interface set `ENABLE_ONEMKL` to `ON` and `ONEMKL_DIR` to the oneMKL installation path.

SUNDIALS has been tested with oneMKL version 2021.4.

11.1.4.11 Building with CUDA

The NVIDIA CUDA Toolkit provides a development environment for GPU-accelerated computing with NVIDIA GPUs. The CUDA Toolkit and compatible NVIDIA drivers are available from the NVIDIA developer website.

To enable CUDA, set `ENABLE_CUDA` to `ON`. If CUDA is installed in a nonstandard location, you may be prompted to set the variable `CUDA_TOOLKIT_ROOT_DIR` with your CUDA Toolkit installation path. To enable CUDA examples, set `EXAMPLES_ENABLE_CUDA` to `ON`.

SUNDIALS has been tested with the CUDA toolkit versions 10 and 11.

11.1.4.12 Building with HIP

HIP(heterogeneous-compute interface for portability) allows developers to create portable applications for AMD and NVIDIA GPUs. HIP can be obtained from HIP GitHub repository.

To enable HIP, set `ENABLE_HIP` to `ON` and set `AMDGPU_TARGETS` to the desired target(ex. gfx705). In addition, set `CMAKE_C_COMPILER` and `CMAKE_CXX_COMPILER` to point to an installation of `hipcc`.

SUNDIALS has been tested with HIP versions between 5.0.0 to 5.4.3.

11.1.4.13 Building with RAJA

RAJA is a performance portability layer developed by Lawrence Livermore National Laboratory and can be obtained from the RAJA GitHub repository.

Building SUNDIALS RAJA modules requires a CUDA, HIP, or SYCL enabled RAJA installation. To enable RAJA, set `ENABLE_RAJA` to `ON`, set `SUNDIALS_RAJA_BACKENDS` to the desired backend (`CUDA`, `HIP`, or `SYCL`), and set `ENABLE_-CUDA`, `ENABLE_HIP`, or `ENABLE_SYCL` to `ON` depending on the selected backend. If RAJA is installed in a nonstandard location you will be prompted to set the variable `RAJA_DIR` with the path to the RAJA CMake configuration file. To enable building the RAJA examples set `EXAMPLES_ENABLE_CXX` to `ON`.

SUNDIALS has been tested with RAJA version 0.14.0.

11.1.4.14 Building with XBraid

XBraid is parallel-in-time library implementing an optimal-scaling multigrid reduction in time (MGRIT) solver. The library is developed by Lawrence Livermore National Laboratory and is available from the XBraid GitHub repository.

To enable XBraid support, set `ENABLE_XBRAID` to `ON`, set `XBRAID_DIR` to the root install location of XBraid or the location of the clone of the XBraid repository.

Note: At this time the XBraid types `braid_Int` and `braid_Real` are hard-coded to `int` and `double` respectively. As such SUNDIALS must be configured with `SUNDIALS_INDEX_SIZE` set to `32` and `SUNDIALS_PRECISION` set to `double`. Additionally, SUNDIALS must be configured with `ENABLE_MPI` set to `ON`.

SUNDIALS has been tested with XBraid version 3.0.0.

11.1.5 Testing the build and installation

If SUNDIALS was configured with `EXAMPLES_ENABLE_<language>` options to `ON`, then a set of regression tests can be run after building with the `make` command by running:

```
% make test
```

Additionally, if `EXAMPLES_INSTALL` was also set to `ON`, then a set of smoke tests can be run after installing with the `make install` command by running:

```
% make test_install
```

11.1.6 Building and Running Examples

Each of the SUNDIALS solvers is distributed with a set of examples demonstrating basic usage. To build and install the examples, set at least of the `EXAMPLES_ENABLE_<language>` options to `ON`, and set `EXAMPLES_INSTALL` to `ON`. Specify the installation path for the examples with the variable `EXAMPLES_INSTALL_PATH`. CMake will generate `CMakeLists.txt` configuration files (and `Makefile` files if on Linux/Unix) that reference the *installed* SUNDIALS headers and libraries.

Either the `CMakeLists.txt` file or the traditional `Makefile` may be used to build the examples as well as serve as a template for creating user developed solutions. To use the supplied `Makefile` simply run `make` to compile and generate the executables. To use CMake from within the installed example directory, run `cmake` (or `ccmake` or `cmake-gui` 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.

11.1.7 Configuring, building, and installing on Windows

CMake can also be used to build SUNDIALS on Windows. To build SUNDIALS for use with Visual Studio the following steps should be performed:

1. Unzip the downloaded tar file(s) into a directory. This will be the `SOLVERDIR`

2. Create a separate `BUILDDIR`

3. Open a Visual Studio Command Prompt and cd to `BUILDDIR`

4. Run `cmake-gui ../SOLVERDIR`

   a. Hit Configure

   b. Check/Uncheck solvers to be built

   c. Change `CMAKE_INSTALL_PREFIX` to `INSTDIR`

   d. Set other options as desired

   e. Hit Generate

5. Back in the VS Command Window:

   a. Run `msbuild ALL_BUILD.vcxproj`

   b. Run `msbuild INSTALL.vcxproj`

The resulting libraries will be in the `INSTDIR`.

The SUNDIALS project can also now be opened in Visual Studio. Double click on the `ALL_BUILD.vcxproj` file to open the project. Build the whole *solution* to create the SUNDIALS libraries. To use the SUNDIALS libraries in your own projects, you must set the include directories for your project, add the SUNDIALS libraries to your project solution, and set the SUNDIALS libraries as dependencies for your project.

11.2 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 the table below. The file extension `.LIB` is typically `.so` for shared libraries and `.a` for static libraries. Note that, in this table 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., `sunlinsol_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.

11.2.1 Using SUNDIALS as a Third Party Library in other CMake Projects

The `make install` command will also install a CMake package configuration file that other CMake projects can load to get all the information needed to build against SUNDIALS. In the consuming project's CMake code, the `find_-package` command may be used to search for the configuration file, which will be installed to `instdir/SUNDIALS_-INSTALL_CMAKEDIR/SUNDIALSConfig.cmake` alongside a package version file `instdir/SUNDIALS_INSTALL_-CMAKEDIR/SUNDIALSConfigVersion.cmake`. Together these files contain all the information the consuming project needs to use SUNDIALS, including exported CMake targets. The SUNDIALS exported CMake targets follow the same naming convention as the generated library binaries, e.g. the exported target for CVODE is `SUNDIALS::cvode`. The CMake code snipped below shows how a consuming project might leverage the SUNDIALS package configuration file to build against SUNDIALS in their own CMake project.

```
project(MyProject)

# Set the variable SUNDIALS_DIR to the SUNDIALS instdir.
# When using the cmake CLI command, this can be done like so:
#   cmake -D SUNDIALS_DIR=/path/to/sundials/installation

find_package(SUNDIALS REQUIRED)

add_executable(myexec main.c)

# Link to SUNDIALS libraries through the exported targets.
# This is just an example, users should link to the targets appropriate
# for their use case.
target_link_libraries(myexec PUBLIC SUNDIALS::cvode SUNDIALS::nvecpetsc)
```

Table 11.1: SUNDIALS shared libraries and header files

Shared	Headers	sundials/sundials_band.h
		sundials/sundials_config.h
		sundials/sundials_context.h
		sundials/sundials_cuda_policies.hpp
		sundials/sundials_dense.h
		sundials/sundials_direct.h
		sundials/sundials_hip_policies.hpp
		sundials/sundials_iterative.h
		sundials/sundials_linearsolver.h
		sundials/sundials_math.h
		sundials/sundials_matrix.h
		sundials/sundials_memory.h
		sundials/sundials_mpi_types.h
		sundials/sundials_nonlinearsolver.h
		sundials/sundials_nvector.h
		sundials/sundials_types.h
		sundials/sundials_version.h
		sundials/sundials_xbraid.h
NVECTOR Modules		
SERIAL	Libraries	libsundials_nvecserial.LIB
	Headers	nvector/nvector_serial.h
PARALLEL	Libraries	libsundials_nvecparallel.LIB
	Headers	nvector/nvector_parallel.h

continues on next page

Table 11.1 – continued from previous page

OPENMP	Libraries	`libsundials_nvecopenmp.LIB`
	Headers	`nvector/nvector_openmp.h`
PTHREADS	Libraries	`libsundials_nvecpthreads.LIB`
	Headers	`nvector/nvector_pthreads.h`
PARHYP	Libraries	`libsundials_nvecparhyp.LIB`
	Headers	`nvector/nvector_parhyp.h`
PETSC	Libraries	`libsundials_nvecpetsc.LIB`
	Headers	`nvector/nvector_petsc.h`
CUDA	Libraries	`libsundials_nveccuda.LIB`
	Headers	`nvector/nvector_cuda.h`
HIP	Libraries	`libsundials_nvechip.LIB`
	Headers	`nvector/nvector_hip.h`
RAJA	Libraries	`libsundials_nveccudaraja.LIB`
		`libsundials_nvechipraja.LIB`
	Headers	`nvector/nvector_raja.h`
SYCL	Libraries	`libsundials_nvecsycl.LIB`
	Headers	`nvector/nvector_sycl.h`
MANYVECTOR	Libraries	`libsundials_nvecmanyvector.LIB`
	Headers	`nvector/nvector_manyvector.h`
MPIMANYVECTOR	Libraries	`libsundials_nvecmpimanyvector.LIB`
	Headers	`nvector/nvector_mpimanyvector.h`
MPIPLUSX	Libraries	`libsundials_nvecmpiplusx.LIB`
	Headers	`nvector/nvector_mpiplusx.h`
SUNMATRIX Modules		
BAND	Libraries	`libsundials_sunmatrixband.LIB`
	Headers	`sunmatrix/sunmatrix_band.h`
CUSPARSE	Libraries	`libsundials_sunmatrixcusparse.LIB`
	Headers	`sunmatrix/sunmatrix_cusparse.h`
DENSE	Libraries	`libsundials_sunmatrixdense.LIB`
	Headers	`sunmatrix/sunmatrix_dense.h`
Ginkgo	Headers	`sunmatrix/sunmatrix_ginkgo.hpp`
MAGMADENSE	Libraries	`libsundials_sunmatrixmagmadense.LIB`
	Headers	`sunmatrix/sunmatrix_magmadense.h`
ONEMKLDENSE	Libraries	`libsundials_sunmatrixonemkldense.LIB`
	Headers	`sunmatrix/sunmatrix_onemkldense.h`
SPARSE	Libraries	`libsundials_sunmatrixsparse.LIB`
	Headers	`sunmatrix/sunmatrix_sparse.h`
SLUNRLOC	Libraries	`libsundials_sunmatrixslunrloc.LIB`
	Headers	`sunmatrix/sunmatrix_slunrloc.h`
SUNLINSOL Modules		
BAND	Libraries	`libsundials_sunlinsolband.LIB`
	Headers	`sunlinsol/sunlinsol_band.h`
CUSOLVERSP_BATCHQR	Libraries	`libsundials_sunlinsolcusolversp.LIB`
	Headers	`sunlinsol/sunlinsol_cusolversp_batchqr.h`
DENSE	Libraries	`libsundials_sunlinsoldense.LIB`
	Headers	`sunlinsol/sunlinsol_dense.h`
Ginkgo	Headers	`sunlinsol/sunlinsol_ginkgo.hpp`
KLU	Libraries	`libsundials_sunlinsolklu.LIB`
	Headers	`sunlinsol/sunlinsol_klu.h`
LAPACKBAND	Libraries	`libsundials_sunlinsollapackband.LIB`
	Headers	`sunlinsol/sunlinsol_lapackband.h`

Table 11.1 – continued from previous page

LAPACKDENSE	Libraries	libsundials_sunlinsollapackdense.LIB
	Headers	sunlinsol/sunlinsol_lapackdense.h
MAGMADENSE	Libraries	libsundials_sunlinsolmagmadense.LIB
	Headers	sunlinsol/sunlinsol_magmadense.h
ONEMKLDENSE	Libraries	libsundials_sunlinsolonemkldense.LIB
	Headers	sunlinsol/sunlinsol_onemkldense.h
PCG	Libraries	libsundials_sunlinsolpcg.LIB
	Headers	sunlinsol/sunlinsol_pcg.h
SPBCGS	Libraries	libsundials_sunlinsolspbcgs.LIB
	Headers	sunlinsol/sunlinsol_spbcgs.h
SPFGMR	Libraries	libsundials_sunlinsolspfgmr.LIB
	Headers	sunlinsol/sunlinsol_spfgmr.h
SPGMR	Libraries	libsundials_sunlinsolspgmr.LIB
	Headers	sunlinsol/sunlinsol_spgmr.h
SPTFQMR	Libraries	libsundials_sunlinsolsptfqmr.LIB
	Headers	sunlinsol/sunlinsol_sptfqmr.h
SUPERLUDIST	Libraries	libsundials_sunlinsolsuperludist.LIB
	Headers	sunlinsol/sunlinsol_superludist.h
SUPERLUMT	Libraries	libsundials_sunlinsolsuperlumt.LIB
	Headers	sunlinsol/sunlinsol_superlumt.h
SUNNONLINSOL Modules		
NEWTON	Libraries	libsundials_sunnonlinsolnewton.LIB
	Headers	sunnonlinsol/sunnonlinsol_newton.h
FIXEDPOINT	Libraries	libsundials_sunnonlinsolfixedpoint.LIB
	Headers	sunnonlinsol/sunnonlinsol_fixedpoint.h
PETSCSNES	Libraries	libsundials_sunnonlinsolpetscsnes.LIB
	Headers	sunnonlinsol/sunnonlinsol_petscsnes.h
SUNMEMORY Modules		
SYSTEM	Libraries	libsundials_sunmemsys.LIB
	Headers	sunmemory/sunmemory_system.h
CUDA	Libraries	libsundials_sunmemcuda.LIB
	Headers	sunmemory/sunmemory_cuda.h
HIP	Libraries	libsundials_sunmemhip.LIB
	Headers	sunmemory/sunmemory_hip.h
SYCL	Libraries	libsundials_sunmemsycl.LIB
	Headers	sunmemory/sunmemory_sycl.h
SUNDIALS Packages		
CVODE	Libraries	libsundials_cvode.LIB
	Headers	cvode/cvode.h
		cvode/cvode_bandpre.h
		cvode/cvode_bbdpre.h
		cvode/cvode_diag.h
		cvode/cvode_direct.h
		cvode/cvode_impl.h
		cvode/cvode_ls.h
		cvode/cvode_proj.h
		cvode/cvode_spils.h
CVODES	Libraries	libsundials_cvodes.LIB
	Headers	cvodes/cvodes.h
		cvodes/cvodes_bandpre.h
		cvodes/cvodes_bbdpre.h

Table 11.1 – continued from previous page

		cvodes/cvodes_diag.h
		cvodes/cvodes_direct.h
		cvodes/cvodes_impl.h
		cvodes/cvodes_ls.h
		cvodes/cvodes_spils.h
ARKODE	Libraries	libsundials_arkode.LIB
		libsundials_xbraid.LIB
	Headers	arkode/arkode.h
		arkode/arkode_arkstep.h
		arkode/arkode_bandpre.h
		arkode/arkode_bbdpre.h
		arkode/arkode_butcher.h
		arkode/arkode_butcher_dirk.h
		arkode/arkode_butcher_erk.h
		arkode/arkode_erkstep.h
		arkode/arkode_impl.h
		arkode/arkode_ls.h
		arkode/arkode_mristep.h
		arkode/arkode_xbraid.h
IDA	Libraries	libsundials_ida.LIB
	Headers	ida/ida.h
		ida/ida_bbdpre.h
		ida/ida_direct.h
		ida/ida_impl.h
		ida/ida_ls.h
		ida/ida_spils.h
IDAS	Libraries	libsundials_idas.LIB
	Headers	idas/idas.h
		idas/idas_bbdpre.h
		idas/idas_direct.h
		idas/idas_impl.h
		idas/idas_spils.h
KINSOL	Libraries	libsundials_kinsol.LIB
	Headers	kinsol/kinsol.h
		kinsol/kinsol_bbdpre.h
		kinsol/kinsol_direct.h
		kinsol/kinsol_impl.h
		kinsol/kinsol_ls.h
		kinsol/kinsol_spils.h

Chapter 12

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. Table 12.1 contains the CVODE input constants, and Table 12.2 contains the CVODE output constants.

Table 12.1: CVODE input constants

`CV_ADAMS`	1	Adams-Moulton linear multistep method.
`CV_BDF`	2	BDF linear multistep method.
`CV_NORMAL`	1	Solver returns at specified output time.
`CV_ONE_STEP`	2	Solver returns after each successful step.
`SUN_PREC_NONE`	0	No preconditioning
`SUN_PREC_LEFT`	1	Preconditioning on the left only.
`SUN_PREC_RIGHT`	2	Preconditioning on the right only.
`SUN_PREC_BOTH`	3	Preconditioning on both the left and the right.
`SUN_MODIFIED_GS`	1	Use modified Gram-Schmidt procedure.
`SUN_CLASSICAL_GS`	2	Use classical Gram-Schmidt procedure.

Table 12.2: CVODE output constants

General outputs		
`CV_SUCCESS`	0	Successful function return.
`CV_TSTOP_RETURN`	1	CVode succeeded by reaching the specified stopping point.
`CV_ROOT_RETURN`	2	CVode succeeded and found one or more roots.
`CV_WARNING`	99	CVode succeeded but an unusual situation occurred.
`CV_TOO_MUCH_WORK`	-1	The solver took `mxstep` internal steps but could not reach tout.
`CV_TOO_MUCH_ACC`	-2	The solver could not satisfy the accuracy demanded by the user for some internal step.
`CV_ERR_FAILURE`	-3	Error test failures occurred too many times during one internal time step or minimum step size was reached.
`CV_CONV_FAILURE`	-4	Convergence test failures occurred too many times during one internal time step or minimum step size was reached.
`CV_LINIT_FAIL`	-5	The linear solver's initialization function failed.
`CV_LSETUP_FAIL`	-6	The linear solver's setup function failed in an unrecoverable manner.
`CV_LSOLVE_FAIL`	-7	The linear solver's solve function failed in an unrecoverable manner.
`CV_RHSFUNC_FAIL`	-8	The right-hand side function failed in an unrecoverable manner.
`CV_FIRST_RHSFUNC_ERR`	-9	The right-hand side function failed at the first call.

continues on next page

Table 12.2 – continued from previous page

CV_REPTD_RHSFUNC_ERR	-10	The right-hand side function had repetead recoverable errors.
CV_UNREC_RHSFUNC_ERR	-11	The right-hand side function had a recoverable error, but no recovery is possible.
CV_RTFUNC_FAIL	-12	The rootfinding function failed in an unrecoverable manner.
CV_NLS_INIT_FAIL	-13	The nonlinear solver's init routine failed.
CV_NLS_SETUP_FAIL	-14	The nonlinear solver's setup routine failed.
CV_CONSTR_FAIL	-15	The inequality constraints were violated and the solver was unable to recover.
CV_NLS_FAIL	-16	The nonlinear solver failed in an unrecoverable manner.
CV_MEM_FAIL	-20	A memory allocation failed.
CV_MEM_NULL	-21	The cvode_mem argument was NULL.
CV_ILL_INPUT	-22	One of the function inputs is illegal.
CV_NO_MALLOC	-23	The CVODE memory block was not allocated by a call to CVodeMalloc.
CV_BAD_K	-24	The derivative order k is larger than the order used.
CV_BAD_T	-25	The time t is outside the last step taken.
CV_BAD_DKY	-26	The output derivative vector is NULL.
CV_TOO_CLOSE	-27	The output and initial times are too close to each other.
CV_VECTOROP_ERR	-28	A vector operation failed.
CV_PROJ_MEM_NULL	-29	The projection memory was NULL.
CV_PROJFUNC_FAIL	-30	The projection function failed in an unrecoverable manner.
CV_REPTD_PROJFUNC_ERR	-31	The projection function had repeated recoverable errors.
CVLS linear solver interface outputs		
CVLS_SUCCESS	0	Successful function return.
CVLS_MEM_NULL	-1	The cvode_mem argument was NULL.
CVLS_LMEM_NULL	-2	The CVLS linear solver has not been initialized.
CVLS_ILL_INPUT	-3	The CVLS solver is not compatible with the current N_Vector module.
CVLS_MEM_FAIL	-4	A memory allocation request failed.
CVLS_PMEM_NULL	-5	The preconditioner module has not been initialized.
CVLS_JACFUNC_UNRECVR	-6	The Jacobian function failed in an unrecoverable manner.
CVLS_JACFUNC_RECVR	-7	The Jacobian function had a recoverable error.
CVLS_SUNMAT_FAIL	-8	An error occurred with the current {sunmatrix} module.
CVLS_SUNLS_FAIL	-9	An error occurred with the current {sunlinsol} module.
CVDIAG linear solver outputs		
CVDIAG_SUCCESS	0	Successful function return.
CVDIAG_MEM_NULL	-1	The cvode_mem argument was NULL.
CVDIAG_LMEM_NULL	-2	The CVDIAG linear solver has not been initialized.
CVDIAG_ILL_INPUT	-3	The CVDIAG solver is not compatible with the current N_Vector module.
CVDIAG_MEM_FAIL	-4	A memory allocation request failed.
CVDIAG_INV_FAIL	-5	A diagonal element of the Jacobian was 0.
CVDIAG_RHSFUNC_UNRECVR	-6	The right-hand side function failed in an unrecoverable manner.
CVDIAG_RHSFUNC_RECVR	-7	The right-hand side function had a recoverable error.

Chapter 13

Release History

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Dec 2023	6.7.0	5.7.0	6.7.0	6.7.0	6.7.0	5.7.0	6.7.0
Nov 2023	6.6.2	5.6.2	6.6.2	6.6.2	6.6.2	5.6.2	6.6.2
Sep 2023	6.6.1	5.6.1	6.6.1	6.6.1	6.6.1	5.6.1	6.6.1
Jul 2023	6.6.0	5.6.0	6.6.0	6.6.0	6.6.0	5.6.0	6.6.0
Mar 2023	6.5.1	5.5.1	6.5.1	6.5.1	6.5.1	5.5.1	6.5.1
Dec 2022	6.5.0	5.5.0	6.5.0	6.5.0	6.5.0	5.5.0	6.5.0
Oct 2022	6.4.1	5.4.1	6.4.1	6.4.1	6.4.1	5.4.1	6.4.1
Oct 2022	6.4.0	5.4.0	6.4.0	6.4.0	6.4.0	5.4.0	6.4.0
Aug 2022	6.3.0	5.3.0	6.3.0	6.3.0	6.3.0	5.3.0	6.3.0
Apr 2022	6.2.0	5.2.0	6.2.0	6.2.0	6.2.0	5.2.0	6.2.0
Feb 2022	6.1.1	5.1.1	6.1.1	6.1.1	6.1.1	5.1.1	6.1.1
Jan 2022	6.1.0	5.1.0	6.1.0	6.1.0	6.1.0	5.1.0	6.1.0
Dec 2021	6.0.0	5.0.0	6.0.0	6.0.0	6.0.0	5.0.0	6.0.0
Sep 2021	5.8.0	4.8.0	5.8.0	5.8.0	5.8.0	4.8.0	5.8.0
Jan 2021	5.7.0	4.7.0	5.7.0	5.7.0	5.7.0	4.7.0	5.7.0
Dec 2020	5.6.1	4.6.1	5.6.1	5.6.1	5.6.1	4.6.1	5.6.1
Dec 2020	5.6.0	4.6.0	5.6.0	5.6.0	5.6.0	4.6.0	5.6.0
Oct 2020	5.5.0	4.5.0	5.5.0	5.5.0	5.5.0	4.5.0	5.5.0
Sep 2020	5.4.0	4.4.0	5.4.0	5.4.0	5.4.0	4.4.0	5.4.0
May 2020	5.3.0	4.3.0	5.3.0	5.3.0	5.3.0	4.3.0	5.3.0
Mar 2020	5.2.0	4.2.0	5.2.0	5.2.0	5.2.0	4.2.0	5.2.0
Jan 2020	5.1.0	4.1.0	5.1.0	5.1.0	5.1.0	4.1.0	5.1.0
Oct 2019	5.0.0	4.0.0	5.0.0	5.0.0	5.0.0	4.0.0	5.0.0
Feb 2019	4.1.0	3.1.0	4.1.0	4.1.0	4.1.0	3.1.0	4.1.0
Jan 2019	4.0.2	3.0.2	4.0.2	4.0.2	4.0.2	3.0.2	4.0.2
Dec 2018	4.0.1	3.0.1	4.0.1	4.0.1	4.0.1	3.0.1	4.0.1
Dec 2018	4.0.0	3.0.0	4.0.0	4.0.0	4.0.0	3.0.0	4.0.0
Oct 2018	3.2.1	2.2.1	3.2.1	3.2.1	3.2.1	2.2.1	3.2.1
Sep 2018	3.2.0	2.2.0	3.2.0	3.2.0	3.2.0	2.2.0	3.2.0
Jul 2018	3.1.2	2.1.2	3.1.2	3.1.2	3.1.2	2.1.2	3.1.2
May 2018	3.1.1	2.1.1	3.1.1	3.1.1	3.1.1	2.1.1	3.1.1
Nov 2017	3.1.0	2.1.0	3.1.0	3.1.0	3.1.0	2.1.0	3.1.0
Sep 2017	3.0.0	2.0.0	3.0.0	3.0.0	3.0.0	2.0.0	3.0.0
Sep 2016	2.7.0	1.1.0	2.9.0	2.9.0	2.9.0	1.3.0	2.9.0

Table 13.1 – continued from previous page

Date	SUNDIALS	ARKODE	CVODE	CVODES	IDA	IDAS	KINSOL
Aug 2015	2.6.2	1.0.2	2.8.2	2.8.2	2.8.2	1.2.2	2.8.2
Mar 2015	2.6.1	1.0.1	2.8.1	2.8.1	2.8.1	1.2.1	2.8.1
Mar 2015	2.6.0	1.0.0	2.8.0	2.8.0	2.8.0	1.2.0	2.8.0
Mar 2012	2.5.0	–	2.7.0	2.7.0	2.7.0	1.1.0	2.7.0
May 2009	2.4.0	–	2.6.0	2.6.0	2.6.0	1.0.0	2.6.0
Nov 2006	2.3.0	–	2.5.0	2.5.0	2.5.0	–	2.5.0
Mar 2006	2.2.0	–	2.4.0	2.4.0	2.4.0	–	2.4.0
May 2005	2.1.1	–	2.3.0	2.3.0	2.3.0	–	2.3.0
Apr 2005	2.1.0	–	2.3.0	2.2.0	2.3.0	–	2.3.0
Mar 2005	2.0.2	–	2.2.2	2.1.2	2.2.2	–	2.2.2
Jan 2005	2.0.1	–	2.2.1	2.1.1	2.2.1	–	2.2.1
Dec 2004	2.0.0	–	2.2.0	2.1.0	2.2.0	–	2.2.0
Jul 2002	1.0.0	–	2.0.0	1.0.0	2.0.0	–	2.0.0
Mar 2002	–	–	1.0.0 [3]	–	–	–	–
Feb 1999	–	–	–	–	1.0.0 [4]	–	–
Aug 1998	–	–	–	–	–	–	1.0.0 [5]
Jul 1997	–	–	1.0.0 [2]	–	–	–	–
Sep 1994	–	–	1.0.0 [1]	–	–	–	–

1. CVODE written

2. PVODE written

3. CVODE and PVODE combined

4. IDA written

5. KINSOL written

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